Horizon 2020

Call: H2020-INFRAIA-2016-2017

(Integrating and opening research infrastructures of European interest)

Topic: INFRAIA-02-2017

Type of action: RIA

(Research and Innovation action)

Proposal number: 731010-1

Proposal acronym: Sumo-Chem

Deadline Id: H2020-INFRAIA-2017-1-two-stage

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How to fill in the forms

The administrative forms must be filled in for each proposal using the templates available in the submission system. Some data fields in the administrative forms are pre-filled based on the previous steps in the submission wizard.

Proposal ID **731010-1** *Acronym* **Sumo-Chem**

1 - General information

Topic	INFRAIA-02-2017
Call Identifier	H2020-INFRAIA-2016-2017
Type of Action	RIA
Deadline Id	H2020-INFRAIA-2017-1-two-stage

Acronym: Sumo-Chem

Proposal title*: Supporting Research in Computational and Experimental Chemistry via Research Infrastructure

Note that for technical reasons, the following characters are not accepted in the Proposal Title and will be removed: < > " &

Duration in months: *36*

Fixed keyword 1: *Knowledge infrastructure* Add

Free keywords: *Computational and Experimental Chemistry, research facility, e-infrastructure resources, metadata, ontology, provenance*

Abstract

The Chemistry community is one of the oldest research communities but it is a starting community with respect to this call because first, it has never had an EU e-infrastructure project as a community; second, it does not have its own ESFRI initiative. Currently there are isolated "islands" of research facilities and e-infrastructure resources that are not available for the whole community. This project will integrate research facilities and infrastructures with computing and data resources into the Sumo-Chem RI to enable joint research involving Computational and Experimental Chemistry and other research communities. This RI will have an open architecture to allow its extension with further research facilities and resources to be used by the Chemistry and other communities. The Sumo-Chem RI will allow researchers and developers to run industrial simulations and scientific experiments using European, regional and national research facilities and e-infrastructure resources through an intuitive and seamless virtual access considering different levels of their expertise and skills. The major innovation of the project will be in management of scientific data covering the whole lifecycle of data using metadata, ontologies and provenance based on advanced data and computing services. Sumo-Chem will enable and support multi-disciplinary research in cooperation with ESFRI and other major research initiatives to address climate and energy societal challenges. The project consortium identified eight scientifically excellent use cases as first users of the Sumo-Chem RI. These use cases well represent the heterogeneity of the Chemistry community.

Remaining characters 338

Has this proposal (or a very similar one) been submitted in the past 2 years in response to a call for proposals under the 7th Framework Programme, Horizon 2020 or any other EU programme(s)? ○ Yes ◉ No

Proposal ID **731010-1** *Acronym* **Sumo-Chem**

Declarations

1) The coordinator declares to have the explicit consent of all applicants on their participation and on the content of this proposal.	☒
2) The information contained in this proposal is correct and complete.	☒
3) This proposal complies with ethical principles (including the highest standards of research integrity — as set out, for instance, in the European Code of Conduct for Research Integrity — and including, in particular, avoiding fabrication, falsification, plagiarism or other research misconduct).	☒

4) The coordinator confirms:

- to have carried out the self-check of the financial capacity of the organisation on http://ec.europa.eu/research/participants/portal/desktop/en/organisations/lfv.html or to be covered by a financial viability check in an EU project for the last closed financial year. Where the result was "weak" or "insufficient", the coordinator confirms being aware of the measures that may be imposed in accordance with the H2020 Grants Manual (Chapter on Financial capacity check); or	○
- is exempt from the financial capacity check being a public body including international organisations, higher or secondary education establishment or a legal entity, whose viability is guaranteed by a Member State or associated country, as defined in the H2020 Grants Manual (Chapter on Financial capacity check); or	◉
- as sole participant in the proposal is exempt from the financial capacity check.	○

5) The coordinator hereby declares that each applicant has confirmed:

- they are fully eligible in accordance with the criteria set out in the specific call for proposals; and	☒
- they have the financial and operational capacity to carry out the proposed action.	☒

The coordinator is only responsible for the correctness of the information relating to his/her own organisation. Each applicant remains responsible for the correctness of the information related to him/her and declared above. Where the proposal to be retained for EU funding, the coordinator and each beneficiary applicant will be required to present a formal declaration in this respect.

According to Article 131 of the Financial Regulation of 25 October 2012 on the financial rules applicable to the general budget of the Union (Official Journal L 298 of 26.10.2012, p. 1) and Article 145 of its Rules of Application (Official Journal L 362, 31.12.2012, p.1) applicants found guilty of misrepresentation may be subject to administrative and financial penalties under certain conditions.

Personal data protection

Your reply to the grant application will involve the recording and processing of personal data (such as your name, address and CV), which will be processed pursuant to Regulation (EC) No 45/2001 on the protection of individuals with regard to the processing of personal data by the Community institutions and bodies and on the free movement of such data. Unless indicated otherwise, your replies to the questions in this form and any personal data requested are required to assess your grant application in accordance with the specifications of the call for proposals and will be processed solely for that purpose. Details concerning the processing of your personal data are available on the privacy statement. Applicants may lodge a complaint about the processing of their personal data with the European Data Protection Supervisor at any time.

Your personal data may be registered in the Early Warning System (EWS) only or both in the EWS and Central Exclusion Database (CED) by the Accounting Officer of the Commission, should you be in one of the situations mentioned in:
-the Commission Decision 2008/969 of 16.12.2008 on the Early Warning System (for more information see the Privacy Statement), or
-the Commission Regulation 2008/1302 of 17.12.2008 on the Central Exclusion Database (for more information see the Privacy Statement) .

Proposal ID **731010-1** *Acronym* **Sumo-Chem**

List of participants

#	Participant Legal Name	Country
1	THE UNIVERSITY OF WESTMINSTER LBG	United Kingdom
2	EBERHARD KARLS UNIVERSITAET TUEBINGEN	Germany
3	MAGYAR TUDOMANYOS AKADEMIA SZAMITASTECHNIKAI ES AUTOMATIZALASI KUTATOINTEZET	Hungary
4	TECHNISCHE UNIVERSITAET DRESDEN	Germany
5	CONSORZIO INTERUNIVERSITARIO CINECA	Italy
6	ELETTRA - SINCROTRONE TRIESTE SCPA	Italy
7	UNIVERSITA DEGLI STUDI DI FIRENZE	Italy
8	CONSIGLIO NAZIONALE DELLE RICERCHE	Italy
9	UNIVERSITA DEGLI STUDI DI PERUGIA	Italy
10	UNIVERSIDAD COMPLUTENSE DE MADRID	Spain
11	UNIVERSIDAD DEL PAIS VASCO/ EUSKAL HERRIKO UNIBERTSITATEA	Spain
12	RHEINISCH-WESTFAELISCHE TECHNISCHE HOCHSCHULE AACHEN	Germany
13	CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE	France
14	AGENZIA NAZIONALE PER LE NUOVE TECNOLOGIE, L'ENERGIA E LO SVILUPPO ECONOMICO SOSTENIBILE	Italy
15	KEMIJSKI INSTITUT	Slovenia
16	RUDER BOSKOVIC INSTITUTE	Croatia
17	Polymechanon	Greece
18	master-up	Italy
19	Blurock Consulting AB	Sweden
20	ECTN Association	Belgium

Proposal ID **731010-1** *Acronym* **Sumo-Chem**

Please provide the complete list of participants to the project and ensure that the eligibility conditions on the composition of the consortium are complied with. Although successful proposals invited to submit a full proposal for the second stage will be allowed to add partners, this may not have the effect of fundamentally altering the proposal submitted for the first stage.

By the complete list of participants, it will be possible to streamline the evaluation process with faster checks for eligibility, and more efficient selection of expert evaluators.

The list of participants is pre-filled based on the information given on Step 4 of the application. To add more partners, please save and close the form and go back to Step 4.

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **UOW**

2 - Administrative data of participating organisations

PIC	***Legal name***
999858250	*THE UNIVERSITY OF WESTMINSTER LBG*

Short name: UOW

Address of the organisation

Street REGENT STREET 309

Town LONDON

Postcode W1B 2UW

Country United Kingdom

Webpage www.westminster.ac.uk

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... yes

Non-profit ..... yes

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... yes

Research organisation ..... yes

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2013 - no

SME self-assessment ..... unknown

SME validation sme ..... unknown

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE Code: 853 - Higher education

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **UOW**

Department(s) carrying out the proposed work

Department 1

Department name: Centre for Parallel Computing, Dept. of Computer Science ☐ not applicable

☐ Same as organisation address

Street: 115 New Cavendish Street

Town: London

Postcode: W1W 6UW

Country: United Kingdom

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **UOW**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Prof. Sex: (•) Male ( ) Female

First name: **Gabor** Last name: **TERSTYANSZKY**

E-Mail: **terstyg@wmin.ac.uk**

Position in org.: Director of the Centre for Parallel Computing

Department: Centre for Parallel Computing ☐ Same as organisation

☐ Same as organisation address

Street: 115 New Cavendish Street

Town: London Post code: W1W 6UW

Country: United Kingdom

Website: westminster.ac.uk

Phone 1: +442079115000 Phone 2: +447443534119 Fax: *+xxx xxxxxxxxx*

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **EKUT**

PIC	***Legal name***
999991916	*EBERHARD KARLS UNIVERSITAET TUEBINGEN*

Short name: EKUT

Address of the organisation

Street GESCHWISTER-SCHOLL-PLATZ

Town TUEBINGEN

Postcode 72074

Country Germany

Webpage www.uni-tuebingen.de

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... yes

Non-profit ..... yes

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... yes

Research organisation ..... yes

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2011 - no

SME self-assessment ..... unknown

SME validation sme ..... unknown

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE Code: - - Not applicable

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **EKUT**

Department(s) carrying out the proposed work

Department 1

Department name: Bioinformatics ☐ not applicable

☐ Same as organisation address

Street: Sand 14

Town: Tübingen

Postcode: 72076

Country: Germany

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **EKUT**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Dr. Sex: (•) Male ( ) Female

First name: **Jens** Last name: **Krüger**

E-Mail: **krueger@informatik.uni-tuebingen.de**

Position in org.: Habilitand

Department: Bioinformatics [ ] Same as organisation

[ ] Same as organisation address

Street: Sand 14

Town: Tübingen Post code: 72076

Country: Germany

Website: http://abi.inf.uni-tuebingen.de/People/krueger

Phone 1: +49-7071-29-70459 Phone 2: *+xxx xxxxxxxxx* Fax: +49-7071-29-5152

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **MTA SZTAKI**

PIC	***Legal name***
999651252	*MAGYAR TUDOMANYOS AKADEMIA SZAMITASTECHNIKAI ES AUTOMATIZALASI KUTATOINTEZ*

Short name: MTA SZTAKI

Address of the organisation

Street KENDE UTCA 13-17

Town BUDAPEST

Postcode 1111

Country Hungary

Webpage www.sztaki.hu

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... yes

Non-profit ..... yes

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... no

Research organisation ..... yes

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2011 - no

SME self-assessment ..... unknown

SME validation sme ..... unknown

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE Code: 721 - Research and experimental development on natural sciences and engineering

Department(s) carrying out the proposed work

Department 1

Department name: Laboratory of Parallel and Distributed Systems ☐ not applicable

☒ Same as organisation address

Street: KENDE UTCA 13-17

Town: BUDAPEST

Postcode: 1111

Country: Hungary

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **MTA SZTAKI**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Prof. Sex: (•) Male ( ) Female

First name: **Peter** Last name: **Kacsuk**

E-Mail: **kacsuk@sztaki.hu**

Position in org.: Head of Laboratory

Department: Laboratory of Parallel and Distributed Systems ☐ Same as organisation

☒ Same as organisation address

Street: KENDE UTCA 13-17

Town: BUDAPEST Post code: 1111

Country: Hungary

Website: www.sztaki.hu

Phone 1: +361 2796064 Phone 2: +361 3297864 Fax: +361 3297864

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **TUD**

PIC	***Legal name***
999897729	*TECHNISCHE UNIVERSITAET DRESDEN*

Short name: TUD

Address of the organisation

Street HELMHOLTZSTRASSE 10

Town DRESDEN

Postcode 01069

Country Germany

Webpage http://www.tu-dresden.de/

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... yes

Non-profit ..... yes

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... yes

Research organisation ..... no

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2014 - no

SME self-assessment ..... unknown

SME validation sme ..... 2013 - no

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE Code: 853 - Higher education

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **TUD**

Department(s) carrying out the proposed work

Department 1

Department name: Center for Information Services and High Performance Computing ☐ not applicable

☐ Same as organisation address

Street: Zellescher Weg 12-14

Town: Dresden

Postcode: 01069

Country: Germany

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **TUD**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Prof. Sex: (•) Male ( ) Female

First name: **Wolfgang E** Last name: **Nagel**

E-Mail: **wolfgang.nagel@tu-dresden.de**

Position in org.: Head of Department

Department: Center for Information Services and High Performance Computing ☐ Same as organisation

☐ Same as organisation address

Street: Zellescher Weg 12-14

Town: Dresden Post code: 01069

Country: Germany

Website: www.tu-dresden.de/zih

Phone 1: +4935146335450 Phone 2: +xxx xxxxxxxxx Fax: +xxx xxxxxxxxx

Other contact persons

First Name	*Last Name*	*E-mail*	*Phone*
Richard	Grunzke	richard.grunzke@tu-dresden.de	+4935146335448

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **CINECA CONSORZIO INTERUNIVERSITAR**

PIC	***Legal name***
999843409	*CONSORZIO INTERUNIVERSITARIO CINECA*

Short name: CINECA CONSORZIO INTERUNIVERSITARIO

Address of the organisation

Street VIA MAGNANELLI 6/3

Town CASALECCHIO DI RENO BO

Postcode 40033

Country Italy

Webpage www.cineca.it

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... yes

Non-profit ..... yes

International organisation ..... unknown

International organisation of European interest ..... unknown

Secondary or Higher education establishment ..... unknown

Research organisation ..... yes

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 1967 - no

SME self-assessment ..... unknown

SME validation sme ..... unknown

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE Code: 72 - Scientific research and development

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **CINECA CONSORZIO INTERUNIVERSITAR**

Department(s) carrying out the proposed work

Department 1

Department name: SCAI - Super Computing Application and Innovation ☐ not applicable

☒ Same as organisation address

Street: VIA MAGNANELLI 6/3

Town: CASALECCHIO DI RENO BO

Postcode: 40033

Country: Italy

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **CINECA CONSORZIO INTERUNIVERSITAR**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Mrs

Sex: ○ Male ◉ Female

First name: **Elda** Last name: **Rossi**

E-Mail: **e.rossi@cineca.it**

Position in org.: head of HPC user support

Department: SCAI - Super Computing Application and Innovation ☐ Same as organisation

☒ Same as organisation address

Street: VIA MAGNANELLI 6/3

Town: CASALECCHIO DI RENO BO Post code: 40033

Country: Italy

Website: hpc.cineca.it

Phone 1: +390516171515 Phone 2: *+xxx xxxxxxxxx* Fax: *+xxx xxxxxxxxx*

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **ELETTRA - SINCROTRONE TRIESTE SCPA**

PIC	***Legal name***
999589851	*ELETTRA - SINCROTRONE TRIESTE SCPA*

Short name: ELETTRA - SINCROTRONE TRIESTE SCPA

Address of the organisation

Street SS 14 KM 163.5

Town BASOVIZZA TRIESTE

Postcode 34149

Country Italy

Webpage www.elettra.trieste.it

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... no

Non-profit ..... yes

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... no

Research organisation ..... yes

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2007 - no

SME self-assessment ..... unknown

SME validation sme ..... 2007 - no

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE Code: - - Not applicable

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **ELETTRA - SINCROTRONE TRIESTE SCPA**

Department(s) carrying out the proposed work

Department 1

Department name: Beamlines GasPhase, LDM ☐ not applicable

☒ Same as organisation address

Street: SS 14 KM 163.5

Town: BASOVIZZA TRIESTE

Postcode: 34149

Country: Italy

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1**	*Acronym* **Sumo-Chem**	*Short name* **ELETTRA - SINCROTRONE TRIESTE SCPA**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Dr. | Sex: (•) Male ( ) Female

First name: **Robert** | Last name: **Richter**

E-Mail: **robert.richter@elettra.eu**

Position in org.: Senior Scientist

Department: ELETTRA - SINCROTRONE TRIESTE SCPA ☒ Same as organisation

☒ Same as organisation address

Street: SS 14 KM 163.5

Town: BASOVIZZA TRIESTE | Post code: 34149

Country: Italy

Website:

Phone 1: +390403758642 | Phone 2: +xxx xxxxxxxxx | Fax: +xxx xxxxxxxxx

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **UNIFI**

PIC	***Legal name***
999895789	*UNIVERSITA DEGLI STUDI DI FIRENZE*

Short name: UNIFI

Address of the organisation

Street Piazza San Marco 4

Town Florence

Postcode 50121

Country Italy

Webpage http://www.unifi.it

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... yes

Non-profit ..... yes

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... yes

Research organisation ..... yes

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2013 - no

SME self-assessment ..... unknown

SME validation sme ..... unknown

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE Code: 853 - Higher education

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **UNIFI**

Department(s) carrying out the proposed work

Department 1

Department name: Chimica "Ugo Schiff"

☐ not applicable

☐ Same as organisation address

Street: via della Lastruccia 3

Town: Sesto Fiorentino (Firenze)

Postcode: 50019

Country: Italy

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **UNIFI**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Prof. Sex: (•) Male ( ) Female

First name: **Gianni** Last name: **Cardini**

E-Mail: **gianni.cardini@unifi.it**

Position in org.: Full Professor

Department: Chimica "Ugo Schiff" [ ] Same as organisation

[ ] Same as organisation address

Street: via della Lastruccia 3

Town: Sesto Fiorentino (Firenze) Post code: 50019

Country: Italy

Website: www2.unifi.it/chimica

Phone 1: +39 3335213799 Phone 2: +39 0552753072 Fax: *+xxx xxxxxxxxx*

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **CNR**

PIC	***Legal name***
999979500	*CONSIGLIO NAZIONALE DELLE RICERCHE*

Short name: CNR

Address of the organisation

Street PIAZZALE ALDO MORO 7

Town ROMA

Postcode 00185

Country Italy

Webpage www.cnr.it

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... yes

Non-profit ..... yes

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... no

Research organisation ..... yes

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2015 - no

SME self-assessment ..... unknown

SME validation sme ..... 2007 - no

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE Code: 721 - Research and experimental development on natural sciences and engineering

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **CNR**

Department(s) carrying out the proposed work

Department 1

Department name: Istituto di Ricerche sulla Combustione ☐ not applicable

☐ Same as organisation address

Street: Piazzale Tecchio n°80

Town: Napoli

Postcode: 80125

Country: Italy

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **CNR**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Dr. Sex: ○ Male ◉ Female

First name: **Mariarosaria** Last name: **Ceglia de Joannon**

E-Mail: **dejoannon@irc.cnr.it**

Position in org.: Researcher

Department: Istituto di Ricerche sulla Combustione ☐ Same as organisation

☐ Same as organisation address

Street: Piazzale Tecchio n°80

Town: Napoli Post code: 80125

Country: Italy

Website: www.irc.cnr.it

Phone 1: +393286188742 Phone 2: +390812301709 Fax: +390812391709

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **UNIPG**

PIC	***Legal name***
999846319	*UNIVERSITA DEGLI STUDI DI PERUGIA*

Short name: UNIPG

Address of the organisation

Street PIAZZA DELL' UNIVERSITA 1

Town PERUGIA

Postcode 06123

Country Italy

Webpage

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... yes

Non-profit ..... yes

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... yes

Research organisation ..... yes

Legal person ..... yes

Enterprise Data

SME self-declared status ..... unknown

SME self-assessment ..... unknown

SME validation sme ..... unknown

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE Code: 80.4 - Adult & other education

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **UNIPG**

Department(s) carrying out the proposed work

Department 1

Department name: Department of Chemistry, Biology and Biotechnology ☐ not applicable

☐ Same as organisation address

Street: via elce di sotto 8

Town: perugia

Postcode: 06123

Country: Italy

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **UNIPG**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Dr. | Sex: ○ Male ◉ Female

First name: **Maria Noelia** | Last name: **Faginas Lago**

E-Mail: **noelia@dyn.unipg.it**

Position in org.: Researcher

Department: Department of Chemistry, Biology and Biotechnology ☐ Same as organisation

☐ Same as organisation address

Street: via elce di sotto 8

Town: Perugia | Post code: 06123

Country: Italy

Website: http://www.chm.unipg.it

Phone 1: +390755855527 | Phone 2: *+xxx xxxxxxxxx* | Fax: *+xxx xxxxxxxxx*

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **UCM**

PIC	***Legal name***
999874546	*UNIVERSIDAD COMPLUTENSE DE MADRID*

Short name: UCM

Address of the organisation

Street AVENIDA DE SENECA 2

Town MADRID

Postcode 28040

Country Spain

Webpage http://www.ucm.es

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... yes

Non-profit ..... yes

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... yes

Research organisation ..... yes

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2013 - no

SME self-assessment ..... unknown

SME validation sme ..... unknown

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE Code: 853 - Higher education

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **UCM**

Department(s) carrying out the proposed work

Department 1

Department name: Centro de Láseres Ultrarrápidos ☐ not applicable

☐ Same as organisation address

Street: Facultad de Ciencias Quimicas

Town: Madrid

Postcode: 28040

Country: Spain

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **UCM**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Prof. Sex: (•) Male ( ) Female

First name: **Luis** Last name: **Banares**

E-Mail: **lbanares@ucm.es**

Position in org.: Professor

Department: Departamento de Química Física I [ ] Same as organisation

[ ] Same as organisation address

Street: Avenida Complutense s/n

Town: Madrid Post code: 28040

Country: Spain

Website: www.ucm.es/ulc

Phone 1: +34913944228 Phone 2: +34659524351 Fax: +34913944135

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **UPV/EHU**

PIC	***Legal name***
999865234	*UNIVERSIDAD DEL PAIS VASCO/ EUSKAL HERRIKO UNIBERTSITATEA*

Short name: UPV/EHU

Address of the organisation

Street BARRIO SARRIENA S N

Town LEIOA

Postcode 48940

Country Spain

Webpage www.ehu.es

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... yes

Non-profit ..... yes

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... yes

Research organisation ..... yes

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2012 - no

SME self-assessment ..... unknown

SME validation sme ..... unknown

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE Code: 853 - Higher education

Department(s) carrying out the proposed work

Department 1

Department name: Departamento de Quimica Fisica ☐ not applicable

☒ Same as organisation address

Street: BARRIO SARRIENA S N

Town: LEIOA

Postcode: 48940

Country: Spain

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **UPV/EHU**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Prof. Sex: (•) Male ( ) Female

First name: **Ernesto** Last name: **Garcia**

E-Mail: **e.garcia@ehu.es**

Position in org.: Professor

Department: Departamento de Quimica Fisica ☐ Same as organisation

☐ Same as organisation address

Street: Paseo de la Universidad

Town: Vitoria Post code: 48511

Country: Spain

Website:

Phone 1: +34653709940 Phone 2: *+xxx xxxxxxxxx* Fax: *+xxx xxxxxxxxx*

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **RWTH AACHEN**

PIC	***Legal name***
999983962	*RHEINISCH-WESTFAELISCHE TECHNISCHE HOCHSCHULE AACHEN*

Short name: RWTH AACHEN

Address of the organisation

Street TEMPLERGRABEN 55

Town AACHEN

Postcode 52062

Country Germany

Webpage www.rwth-aachen.de

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... yes

Non-profit ..... yes

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... yes

Research organisation ..... yes

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2013 - no

SME self-assessment ..... unknown

SME validation sme ..... 2013 - no

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE Code: 853 - Higher education

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **RWTH AACHEN**

Department(s) carrying out the proposed work

Department 1

Department name: Department of Chemistry, Institute for Inorganic Chemistry ☐ not applicable

☐ Same as organisation address

Street: Landoltweg 1

Town: Aachen

Postcode: 52074

Country: Germany

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **RWTH AACHEN**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Prof. Sex: ○ Male ◉ Female

First name: **Sonja** Last name: **Herres-Pawlis**

E-Mail: **sonja.herres-pawlis@rwth-aachen.de**

Position in org.: Chair of Bioinorganic Chemistry

Department: Department of Chemistry, Institute for Inorganic Chemistry ☐ Same as organisation

☐ Same as organisation address

Street: Landoltweg 1

Town: Aachen Post code: 52074

Country: Germany

Website: http://www.bioac.ac.rwth-aachen.de/

Phone 1: +492418093902 Phone 2: +xxx xxxxxxxxx Fax: +xxx xxxxxxxxx

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **CNRS**

PIC	***Legal name***
999997930	*CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE*

Short name: CNRS

Address of the organisation

Street Rue Michel -Ange 3

Town PARIS

Postcode 75794

Country France

Webpage www.cnrs.fr

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... yes

Non-profit ..... yes

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... no

Research organisation ..... yes

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2013 - no

SME self-assessment ..... unknown

SME validation sme ..... 2013 - no

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE Code: 721 - Research and experimental development on natural sciences and engineering

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **CNRS**

Department(s) carrying out the proposed work

Department 1

Department name: LRGP, Laboratoire Réactions et Génie des Procédés UMR 7274 ☐ not applicable

☐ Same as organisation address

Street: 1 rue Grandville

Town: Nancy

Postcode: 54001

Country: France

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **CNRS**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Dr. Sex: (•) Male ( ) Female

First name: **Frederique** Last name: **Battin-Leclerc**

E-Mail: **frederique.battin-leclerc@univ-lorraine.fr**

Position in org.: Senior Researcher

Department: LRGP, Laboratoire Réactions et Génie des Procédés UMR 7274 ☐ Same as organisation

☐ Same as organisation address

Street: 1 rue Grandville

Town: Nancy Post code: 54001

Country: France

Website: www.lrgp.univ-lorraine.fr

Phone 1: +33383175125 Phone 2: *+xxx xxxxxxxxx* Fax: +33383378120

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **ENEA**

PIC	***Legal name***
999988521	*AGENZIA NAZIONALE PER LE NUOVE TECNOLOGIE, L'ENERGIA E LO SVILUPPO ECONOMICO*

Short name: ENEA

Address of the organisation

Street Lungotevere Grande Ammiraglio Thaon di Reve

Town ROMA

Postcode 00196

Country Italy

Webpage http://www.enea.it

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... yes

Non-profit ..... yes

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... no

Research organisation ..... yes

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2013 - no

SME self-assessment ..... unknown

SME validation sme ..... 2013 - no

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE Code: - - Not applicable

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **ENEA**

Department(s) carrying out the proposed work

Department 1

Department name: Energy Technologies Department, ICT Division ☐ not applicable

☒ Same as organisation address

Street: Lungotevere Grande Ammiraglio Thaon di R

Town: ROMA

Postcode: 00196

Country: Italy

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **ENEA**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Dr. | Sex: (•) Male ( ) Female

First name: **Massimo** | Last name: **Celino**

E-Mail: **massimo.celino@enea.it**

Position in org.: Researcher

Department: Energy Technologies Department, ICT Division | [ ] Same as organisation

[ ] Same as organisation address

Street: Via Anguillarese 301

Town: Rome | Post code: 00123

Country: Italy

Website: www.enea.it

Phone 1: +390630483871 | Phone 2: *+xxx xxxxxxxxx* | Fax: *+xxx xxxxxxxxx*

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **KI**

PIC	***Legal name***
998756718	*KEMIJSKI INSTITUT*

Short name: KI

Address of the organisation

Street HAJDRIHOVA 19

Town LJUBLJANA

Postcode 1000

Country Slovenia

Webpage http://www.ki.si

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... yes

Non-profit ..... yes

International organisation ..... unknown

International organisation of European interest ..... unknown

Secondary or Higher education establishment ..... unknown

Research organisation ..... yes

Legal person ..... yes

Enterprise Data

SME self-declared status..... unknown

SME self-assessment ..... unknown

SME validation sme..... unknown

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE Code: 721 - Research and experimental development on natural sciences and engineering

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **KI**

Department(s) carrying out the proposed work

Department 1

Department name: Laboratory for Biocomputing and Bioinformatics ☐ not applicable

☒ Same as organisation address

Street: HAJDRIHOVA 19

Town: LJUBLJANA

Postcode: 1000

Country: Slovenia

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **KI**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Dr. Sex: (•) Male ( ) Female

First name **Jernej** Last name **Stare**

E-Mail **jernej.stare@ki.si**

Position in org.: Senior Research Associate

Department: Laboratory for Biocomputing and Bioinformatics ☐ Same as organisation

☒ Same as organisation address

Street: HAJDRIHOVA 19

Town: LJUBLJANA Post code: 1000

Country: Slovenia

Website: http://www.ki.si/en/life-sciences/l01-laboratory-for-biocomputing

Phone 1: +386 1 476 0379 Phone 2: +xxx xxxxxxxxx Fax: +386 1 476 0300

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **RBI**

PIC	***Legal name***
999875031	*RUDER BOSKOVIC INSTITUTE*

Short name: RBI

Address of the organisation

Street Bijenicka cesta 54

Town ZAGREB

Postcode 10000

Country Croatia

Webpage www.irb.hr

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... yes

Non-profit ..... yes

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... no

Research organisation ..... yes

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2010 - no

SME self-assessment ..... unknown

SME validation sme ..... unknown

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE Code: - - Not applicable

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **RBI**

Department(s) carrying out the proposed work

Department 1

Department name: Division of Organic Chemistry and Biochemistry ☐ not applicable

☒ Same as organisation address

Street: Bijenicka cesta 54

Town: ZAGREB

Postcode: 10000

Country: Croatia

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **RBI**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Dr. Sex: (•) Male ( ) Female

First name: **Robert** Last name: **Vianello**

E-Mail: **robert.vianello@irb.hr**

Position in org.: Senior Scientist and Group Leader

Department: Division of Organic Chemistry and Biochemistry ☐ Same as organisation

☒ Same as organisation address

Street: Bijenicka cesta 54

Town: ZAGREB Post code: 10000

Country: Croatia

Website: http://www.irb.hr/eng/People/Robert-Vianello

Phone 1: +385 912547100 Phone 2: +385 14561117 Fax: +385 14561118

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **Polymechanon**

PIC	***Legal name***
942746008	*Polymechanon*

Short name: Polymechanon

Address of the organisation

Street Mitropoleos 16

Town Thessaloniki

Postcode 54624

Country Greece

Webpage www.polymechanon.eu

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... no

Non-profit ..... no

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... no

Research organisation ..... no

Legal person ..... no

Enterprise Data

SME self-declared status..... unknown

SME self-assessment ..... unknown

SME validation sme..... unknown

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE Code: 62 - Computer programming, consultancy and related activities

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **Polymechanon**

Department(s) carrying out the proposed work

Department 1

Department name: Research and Development ☐ not applicable

☒ Same as organisation address

Street: Mitropoleos 16

Town: Thessaloniki

Postcode: 54624

Country: Greece

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **Polymechanon**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Dr. Sex: (•) Male ( ) Female

First name: **Ioannis** Last name: **Kozaris**

E-Mail: **ikozaris@chem.auth.gr**

Position in org.: Head

Department: Research and Development ☐ Same as organisation

☒ Same as organisation address

Street: Mitropoleos 16

Town: Thessaloniki Post code: 54624

Country: Greece

Website: www.polymechanon.eu

Phone 1: +302310997704 Phone 2: *+xxx xxxxxxxxx* Fax: *+xxx xxxxxxxxx*

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **master-up**

PIC	***Legal name***
952594127	*master-up*

Short name: master-up

Address of the organisation

Street Via elce di sotto 8

Town perugia

Postcode 06123

Country Italy

Webpage www.master-up.it

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... no

Non-profit ..... no

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... no

Research organisation ..... no

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2011 - yes

SME self-assessment ..... unknown

SME validation sme ..... unknown

Based on the above details of the Beneficiary Registry the organisation is an SME (small- and medium-sized enterprise) for the call.

NACE Code: 72 - Scientific research and development

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **master-up**

Department(s) carrying out the proposed work

Department 1

Department name: Master-up ☐ not applicable

☒ Same as organisation address

Street: Via elce di sotto 8

Town: perugia

Postcode: 06123

Country: Italy

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **master-up**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Prof. Sex: (•) Male ( ) Female

First name: **Antonio** Last name: **Lagana**

E-Mail: **lagana05@gmail.com**

Position in org.: President

Department: master-up ☒ Same as organisation

☒ Same as organisation address

Street: Via elce di sotto 8

Town: perugia Post code: 06123

Country: Italy

Website: www.master-up.it

Phone 1: +393282435094 Phone 2: +xxx xxxxxxxxx Fax: +xxx xxxxxxxxx

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **Blurock Consulting AB**

PIC	***Legal name***
927354824	*Blurock Consulting AB*

Short name: Blurock Consulting AB

Address of the organisation

Street Bandelsvagen 1

Town Lund

Postcode SE-22594

Country Sweden

Webpage http://esblurock.info

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... no

Non-profit ..... no

International organisation ..... no

International organisation of European interest ..... no

Secondary or Higher education establishment ..... no

Research organisation ..... no

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2015 - yes

SME self-assessment ..... 2015 - yes

SME validation sme ..... unknown

Based on the above details of the Beneficiary Registry the organisation is an SME (small- and medium-sized enterprise) for the call.

NACE Code: 7210 - Research and experimental development on natural sciences and engineering

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **Blurock Consulting AB**

Department(s) carrying out the proposed work

Department 1

Department name: Combustion Research ☐ not applicable

☒ Same as organisation address

Street: Bandelsvagen 1

Town: Lund

Postcode: SE-22594

Country: Sweden

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **Blurock Consulting AB**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Dr. Sex: (•) Male ( ) Female

First name: **Edward** Last name: **Blurock**

E-Mail: **edward.blurock@gmail.com**

Position in org.: CEO

Department: Blurock Consulting AB ☒ Same as organisation

☒ Same as organisation address

Street: Bandelsvagen 1

Town: Lund Post code: SE-22594

Country: Sweden

Website: http://esblurock.info/homepage/

Phone 1: +46706633463 Phone 2: +xxx xxxxxxxxx Fax: +xxx xxxxxxxxx

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **ECTN Association**

PIC	***Legal name***
934087691	*ECTN Association*

Short name: ECTN Association

Address of the organisation

Street c/o SEFI, 39, Rue des Deux Eglises

Town Brussels

Postcode 1000

Country Belgium

Webpage www.ectn-assoc.org

Legal Status of your organisation

Research and Innovation legal statuses

Public body ..... no

Non-profit ..... yes

International organisation ..... no

International organisation of European interest ..... yes

Secondary or Higher education establishment ..... no

Research organisation ..... no

Legal person ..... yes

Enterprise Data

SME self-declared status ..... 2014 - no

SME self-assessment ..... unknown

SME validation sme ..... unknown

Based on the above details of the Beneficiary Registry the organisation is not an SME (small- and medium-sized enterprise) for the call.

NACE Code: -

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **ECTN Association**

Department(s) carrying out the proposed work

Department 1

Department name: ECTN Association ☐ not applicable

☒ Same as organisation address

Street: c/o SEFI, 39, Rue des Deux Eglises

Town: Brussels

Postcode: 1000

Country: Belgium

Dependencies with other proposal participants

Character of dependence	***Participant***	

Proposal ID **731010-1** *Acronym* **Sumo-Chem** *Short name* **ECTN Association**

Person in charge of the proposal

The name and e-mail of contact persons are read-only in the administrative form, only additional details can be edited here. To give access rights and basic contact details of contact persons, please go back to Step 4 of the submission wizard and save the changes.

Title: Prof. Sex: (•) Male ( ) Female

First name: **Pavel** Last name: **Drasar**

E-Mail: **pavel.drasar@vscht.cz**

Position in org.: President

Department: ECTN Association ☒ Same as organisation

☐ Same as organisation address

Street: c/o VSCHT Praha, Technicka 5

Town: Praha 6 Post code: 166 28

Country: Czech Republic

Website: http://ectn-assoc.cpe.fr/

Phone 1: +420 602383114 Phone 2: +420443698 Fax: *+xxx xxxxxxxxx*

Proposal ID **731010-1** *Acronym* **Sumo-Chem**

3 - Budget for the proposal

Total requested EU contribution for the proposal/ €	3 811 000

Proposal Information	
Proposal Title	**Supporting Research in Computational and Experimental Chemistry via Research Infrastructure**
Proposal Acronym	**Sumo-Chem**
Type of Funding Scheme	**RIA**
Project Duration	**3 years**
Work Programme Topic addressed	**European Research Infrastructures (including e-Infrastructures)** **INFRAIA-02-2017: Integrating Activities for Starting Communities**
Coordinator Person	**Gabor Terstyanszky**

Participant No	Participant organisation name	Country
1 (coordinator)	University of Westminster	UK
2	University of Tübingen	D
3	Magyar Tudomanyos Akademia Szamitestechnikai Kutato Intezete	H
4	Technische Universität Dresden	D
5	CINECA - Consorzio Interuniversitario	IT
6	Elettra Sincrotrone Trieste	IT
7	Università degli Studi di Firenze	IT
8	Consiglio Nazionale delle Ricerche	IT
9	Università degli Studi di Perugia	IT
10	Universidad Complutense de Madrid	E
11	Universidad del Pais Vasco/Euskal Herriko Unibertsitatea	E
12	Rheinische-Westfaelische Technische Hochschule Aachen	D
13	Centre National de la Recherche Scientifique	F
14	Agenzia Nazionale per le Nuove Technologie, L'Energia e lo Sviluppo Economico Sostenibile	IT
15	Kemijski Institut	SLO
16	Ruder Boskovic Institute	HR
17	Polymechanon	GR
18	Master-up s.r.l.	IT
19	Blurock Consulting AB	SE
20	European Chemistry Thematic Network Association	B

Project summary

The Chemistry community is one of the oldest research communities but it is a starting community with respect to this call because first, it has never had an EU e-infrastructure project as a community; second, it does not have its own ESFRI initiative. Currently there are isolated "islands" of research facilities and e-infrastructure resources that are not available for the whole community. This project will integrate research facilities and infrastructures with computing and data resources into the Sumo-Chem RI to enable joint research involving Computational and Experimental Chemistry and other research communities. This RI will have an open architecture to allow its extension with further research facilities and resources to be used by the Chemistry and other communities. The Sumo-Chem RI will allow researchers and developers to run industrial simulations and scientific experiments using European, regional and national research facilities and e-infrastructure resources through an intuitive and seamless virtual access considering different levels of their expertise and skills. The major innovation of the project will be in management of scientific data covering the whole lifecycle of data using metadata, ontologies and provenance based on advanced data and computing services. Sumo-Chem will enable and support multi-disciplinary research in cooperation with ESFRI and other major research initiatives to address climate and energy societal challenges. The project consortium identified eight scientifically excellent use cases as first users of the Sumo-Chem RI. These use cases well represent the heterogeneity of the Chemistry community.

Table of Contents

1. Excellence

1.1 Objectives

Project aim:

- To integrate research facilities, research infrastructures and e-infrastructure resources into the Sumo-Chem RI to enable joint research involving Computational and Experimental Chemistry and other research communities to address climate and energy societal challenges.

Project objectives:

- To create the Sumo-Chem as an European Research Infrastructure (further RI) to allow researchers and companies running industrial simulations and scientific experiments in Computational and Experimental Chemistry using European, regional and national research facilities and e-infrastructure resources and services.
- To offer intuitive, seamless and virtual access to key European, regional and national research facilities and e-infrastructure resources and services considering different levels of expertise and skills of developers and researchers to run industrial simulations and scientific experiments.
- To support efficient management of scientific data including creating, publishing, accessing, curation, preservation of the data using metadata, ontologies and provenance based on advanced data and computing services.
- To enable and support multi-disciplinary research in cooperation with ESFRI and other major research initiatives to address climate and energy societal challenges.

1.2 Relation to the work programme

Specific Challenge. The project will create the Sumo-Chem RI on European scale opening up key national and regional research facilities and e-infrastructure resources to all European researchers, from both academia and industry ensuring optimal use of RI in development and research.

Scope and theme.

Consortium of several key research infrastructures and **other stakeholders**. The project will create the Sumo-Chem RI to support collaborative development and research in Computational and Experimental Chemistry targeting the climate and energy societal challenge. This RI will involve key European research facilities such as, advanced experimental laboratories and multi-scale accurate complex simulators. It will provide access to these research facilities and to large European computing and data resources to run laboratory experiments, high-performance simulations and exchange data they produce. This RI will provide trans-national and virtual access to research facilities, compute and data resources for both academia and industry. The project consortium will incorporate as stakeholders research facility providers, technology providers, research teams and SMEs from 11 member states.

Access to key European, national and regional research infrastructures. The European Chemistry community, represented by EUCHEMS (Association for Chemical and Molecular Sciences), has about 160,000 members who are either Computational or Experimental Chemists. Considering that more than half of them do research activities there is a large number of prospective users of the Sumo-Chem RI. For example, there are 1000 members of the EUCHEMS Computational Chemistry division, MoSgrid has more than 425 registered users, etc. There is a large pool of European, national and regional facilities and resources in the Chemistry community. They exist as isolated "islands" and many of them are not available for the whole community. The Sumo-Chem RI will open up them for the whole community creating a "continent" of these "islands". This RI will also help exchanging the best practices in the Chemistry community. In doing this they will help addressing societal challenges with particular emphasis on energy efficiency, renewable sources and waste management as focus areas.

Networking, **standardisation** and common **access procedure for trans-national and/or virtual access provision**. The project will provide trans-national and/or virtual access to the Sumo-Chem RI. It will also define access procedures and policies how to use this infrastructure.

Curation, preservation and provision of access to the data. The project will support the whole data life cycle from creating, publishing, accessing, curating and, preserving the data using metadata, ontologies and provenance. Data resources to be used in experiments and simulations will include European, national and regional data resources. Depending on the data resource the RI will provide access to them using either the advanced EUDAT B2xx services or other data access services in cooperation with the e-infrastructure providers through the Sumo-Chem Data Service.

Fostering the potential for innovation of RIs. The project consortium contains SMEs to reinforce the partnership with industry. Developers and researchers of these SMEs will use the Sumo-Chem RI. The project will leverage on the innovative streamlines of these SMEs to foster the development of experimental industrial prototypes. The project will be supported by the Computational Chemistry Division EUCHEMS, European organizations and national associations of Chemists. Sumo-Chem will create an advisory board that will incorporate high level representatives of the European industrial policy makers like the EESC.

Collaboration with ESFRI and other world-class RIs. The project will address the "Secure clean and efficient energy" and "Climate" societal challenge targeting the "Competitive low-carbon energy", "Energy efficiency" and "Waste" focus areas. This project will follow multi-disciplinary research to improve energy efficiency, usage of low-carbon energy, and improve waste management further extending existing and establishing new links with the ESFRI

project ECCSEL (Energy), IAGOS (Environmental Sciences) ELI (Physical Sciences and Engineering). Furthermore Sumo-Chem will work in collaboration with FELs of Europe, the network of European FELs derived from the two ESFRI projects EuroFEL and European XFEL.

1.3 Concept and approach

1.3.1 Background and use cases

Computational and Experimental Chemistry. In recent years, there has been a significant evolution of computational and experimental techniques. Their synergic use has both enabled an accurate determination of intra and intermolecular interactions and offered a rationale for driving molecular processes to produce innovation. The latter has leveraged on the measurement and calculation of detailed structural (electronic energies and molecular geometries) and dynamical (probabilities, cross sections and rate coefficients) properties of elementary chemical processes occurring in gas and in condensed phase. Further studies of the evolution in time of interleaved elementary processes in kinetics, as well as their combination with statistical, fluid dynamics and/or condensed phase treatments, have also led to the accurate modelling of important phenomena and to the development of innovative technological solutions to important societal challenges, such as climate change, green energy, food security, smart cities. The project will create the Sumo-Chem RI to enable a synergetic cooperation between researchers of Computational Chemistry and the related Experimental Chemistry. Computational Chemists will design and implement applications as a service to simulate molecular properties using the computing and data resources of the RI while Experimental Chemists will design and run laboratory experiments aimed at checking the results of the performed simulations using the research facilities of the RI. Their interaction will lead to the design of more advanced experiments and creating more accurate simulations. Moreover it will also lead to development of industrial prototypes. The project selected 8 use cases considering the required research facilities, computing and data services, the addressed societal challenges and the involved multi-disciplinary research. Use case 1-6 and 8 are Chemistry, use case 7 is Energy related use case. Next, we give a short summary of these use cases, research facilities and computing resources to be integrated in the Sumo-Chem, RI..

Use case 1: Chemical dynamics and energetics. This use case will utilize beamlines of the ***Synchrotron*** and ***Free Electron Laser*** light sources to investigate molecular systems interacting with radiation in a wide range of energies, photon field strengths and temporal regimes. These experiments will allow researchers to investigate specific properties of matter under selected conditions. Such experiments generate a large volume of data, with computational chemistry being indispensable for the analysis. Ab initio simulation software packages such as ***ADF, DALTON, MCDTH, NWCHEM, VENUS***, etc. running on high performance computing resources will be used.

Use case 2: Functional and structural properties of matter. It will use ***femtosecond*** and ***nanosecond pulsed lasers*** in combination ***with pump-probe*** and ***laser spectroscopy, time-of-flight mass spectrometry*** and ***ion and photoelectron imaging techniques*** to study the dynamics, stereo-dynamics and quantum control of molecular processes including molecular photo-dissociation and photo-chemistry and bimolecular reactive and inelastic collisions and material science with lasers. Complementary to experiments researchers will run simulations to study the dynamics of elementary molecular processes using electronic structure calculation software (***MOLPRO, MOLCAS, GAUSSIAN***).

Use case 3: Plasma in non-equilibrium conditions. Plasma phenomena in non-equilibrium conditions are currently being experimentally and theoretically studied at the ***Beyond Nano*** RI to obtain an efficient use of energy in different applications. The modelling team complements the experimental investigation of plasma by revealing details impossible or very difficult to access in the experimental approach. To solve Boltzmann transport equations (BTE), deterministic (state-to-state molecular dynamics) and stochastic methods packages such as ***DSMC*** (Direct Simulation Monte Carlo) and ***PIC*** (Particle-in-Cell) will be ported to the RECAS computational infrastructure. The following in-house developed simulation packages: ***PLASMA-FLU*** (plasma simulation), ***PIC, DSMC, EPDA*** (elementary processes data aggregator) will ported to the Sumo-Chem RI.

Use case 4: Spectrum of metal complexes. Experimentalists will record non-linear and time-resolved spectra of metal complexes using ***x-ray absorption, flash laser*** and ***linear and time-resolved spectroscopy*** and compare the results with simulated spectra to find the best matching molecular structure. Computational Chemists will explore the phase space running atomistic simulations for computing free energy surfaces. They will analyse simulation data of metal complexes complementing experiments for vibrational and electronic spectroscopic properties in different environments. There are further simulations related to experiments investigating ground and excited electronic states under controlled conditions of temperature and pressure using linear and time-resolved spectroscopy. These simulations will use*:* ***NWChem, Gaussian, ORCA, Jaguar, MOPAC, DFTB+, MNDO99.***

Use case 5: Renewable energy storage as chemicals. It will leverage on design of complex kinetic systems involving gas and solid state catalysed processes using efficiency parameters derived from ab initio studies checked against highly detailed measurements of the corresponding elementary gas phase processes obtained from ***molecular beam-beam*** and ***beam gas*** experiments. The measurements will also utilise a prototype industrial apparatus, built by a consortium of SMEs coordinated by Master-up, to use energy from renewable sources to produce methane from CO_2 and store it in forms easy and safe to transport. The complex kinetics simulations will make use of the ***ZACROS*** code. The accurate calculations of the dynamical properties will make use of the software packages: ***APH3D*** (both time dependent and time independent), ***ABC, RWAVEPR*** and ***VENUS***.

Use case 6: Cleaner combustion. It will focus on design of smart energy carriers based on COST SMARTCATS to increase fuel flexibility and carbon efficiency of energy production and to support distributed energy generation strategies by bringing together numerical and diagnostic tools. The experimental RI ranges from elementary reactors (***sodium-cooled fast*** and ***plug flow reactor***) and to complex systems (***engine*** and ***cyclonic burners***) enhanced by analytical chemistry techniques (GC/MS, HPLC) and advanced optical diagnostics (**spectroscopic** and ***laser-induced fluorescence - LIF- measurements***). The simulations based on ***CRECK, Pope, ANOVA*** (variance analysis) and ***Tukey*** or ***Dunnett*** modelling software to complement the experiments by validating the experimental results and optimizing the combustion process.

Use case 7: Secure, clean and efficient energy production: low carbon technologies. It will develop market affordable, cost-effective and resource efficient solutions for the energy system based on low-carbon technologies through the CMAST virtual laboratory by designing new materials at the nanoscale level, combining experimental and numerical results and speeding up the production of specialized nanomaterials for energy applications. Computer modelling technologies will be used to reveal the microscopic origin of macroscopic properties and will be exploited for both increasing the efficiency of devices producing and storing energy and for lowering the quantity of needed raw materials. The use case will focus on materials for PV, hydrogen and nuclear technologies in order to enhance their chemical properties at the interface.

Use case 8: Optimization of Biodiesel Production. It will investigate kinetic and thermodynamic parameters of high complexity associated with biodiesel synthesis. The related transesterification reactions involving plant oils and methanol in a strongly alkaline medium will be simulated using QM/MM multi-scale and the Empirical Valence Bond (EVB) method using ***MOLARIS, Q*** and ***GAUSSIAN***. The use case will use computer cluster and ***experimental equipment*** for ***kinetic studies***. The use case fits the societal challenge "Competitive low-carbon energy". The simulations produce large volume of complex and diverse data including experimental kinetic parameters, trajectories and rheological information that requires new protocols for data storage, sharing and analysis.

Research facilities. Analysing the eight use cases the project identified the research facilities and infrastructures, listed in Table 1.1, (where: EU – European, NA – national and RE – regional) used by the Chemistry community and to be integrated in the Sumo-Chem RI. (Remark : We give a description only of the European and National research facilities.)

research facility and infrastructures	Provider	EU	NA	RE	TRL	use cases
ELETTRA synchrotron facility	Elettra Sincrotrone Trieste	X			9	1, 3,4
FERMI free electron laser facility	Elettra Sincrotrone Trieste	X			9	All
non-linear spectroscopy	LENS, Firenze	X			9	1,2,4
FLASH free electron laser	DESY, Hamburg	X			8	1,2,4
PETRA III accelerator	DESY, Hamburg	X			9	4
crossed beams and beam gas facility	Beamlab, Perugia		X		8	2, 3, 5,6
plasma facility	Beyond Nano RI, Bari		X		9	3,5
ultrafast lasers + spectroscopy	CLUR/UCM, Madrid		X		8	2,3,4, 5
shock wave combustion experiments	CNRS, France		X		9	6-7
laboratory burners	CNRS, France		X		9	6-7
Jet-stirred and plug flow reactor	ENSIC, France			X	8	6-7
shock wave spectroscopy	ENSIC, Nancy			X	9	6-7
cyclonic and engine burner	CNR-IRC, Napoli			X	9	6-7
sodium-cooled fast and plug flow reactor	CNR-IRC, Napoli			X	8	5,6-7
experimental kinetics laboratory	Ljubljana			X	8	8
UV/Vis, Raman facilities	Aachen			X	8	4

Table 1.1: Research facilities in the Sumo-Chem RI

Elettra-Sincrotrone Trieste specialized in generating ***synchrotron*** (***Elettra***) and ***free-electron laser*** (***FERMI***) radiation. The two facilities enable the characterization of material properties and functions with sensitivity down to molecular and atomic levels, to pattern and nanofabricate new structures and devices, and to develop new processes. ***Elettra*** provides all of the most important x-ray based techniques in the areas of spectroscopy, spectro microscopy, diffraction, scattering and lithography, as well as providing facilities for infrared microscopy and spectroscopy, ultraviolet inelastic scattering, and band mapping. ***FERMI*** is a single pass seeded FEL light source. Access to Elettra and FERMI will be provided through applications considering scientific merits. **LENS** provides ***short-pulse lasers*** as experimental facilities for spectroscopic and non-linear optics research with frequency domain from the far IR to the extreme UV with the highest available resolution with the time domain from few femto to nanoseconds. They allow running time-resolved spectroscopic experiments such as degenerate and non-degenerate four wave mixing experiments (photon echo, optical Kerr effect, transient gratings, etc.), time resolved fluorescence, two-dimensional infrared spectroscopy, transient absorption and stimulated emission and multi-photon spectroscopy. **FLASH**, the Free-Electron LASer is a ***laser for VUV*** and ***soft X-ray radiation***. It is operated in the "self-amplified spontaneous emission" (SASE) mode and covers a wavelength range from 4.2 nm to about 45 nm in the first harmonic with GW peak power and pulse durations between 50 fs and 200 fs. The **PETRA accelerator** is ***storage ring based X-ray source*** to run pump-probe X-ray absorption experiments with high photon flux in the energy range of 50–150 keV in a 40-bunch mode. **BeamLab**

owns different ***crossed molecular beam and beam gas apparatuses*** in which reactant beam generation and velocity selection coupled with both product mass spectrometric and time of flight analysis and when possible with selective excitation of the transient are employed to investigate single collision processes. **Beyond Nano RI** investigates laser-induced plasma and phenomena under non-equilibrium conditions in order to obtain an efficient use of energy in technological applications, such as negative ion sources for nuclear fusion, material science for aerospace and microelectronics applications, plasma-based energy recovery devices as well as micro-discharges for active flow control, and material synthesis and characterization. **CLUR** runs an RI that provides ***high power pulsed lasers*** in combination with ***multi-photon ionization laser spectroscopy*** and ***time-of-flight mass spectrometry***. These research facilities also allow manipulation of materials (laser micro-fabrication, laser modification of materials, laser ablation) and the study of the dynamics, stereo-dynamics and quantum control of molecular processes. The centre is specialized in the experimental investigated of laser assisted elementary bimolecular processes as well as photo-dissociation and photo-chemistry a Complementary to experiments researchers will run simulations using both quantum and classical mechanics means. **CNRS** has a wide range of research facilities to support extended investigations on ***combustion***. Its facilities support research on the formation and exploitation of oil, the design and implementation of advanced engines, the thermochemical conversion of biomasses.

Computing resources. Complementary to the experiments Computational Chemists run simulations to study the dynamics of elementary and complex molecular processes and structures by means of quantum mechanical and classical methods; and ab initio and density functional electronic molecular structure calculations. The Chemistry community already uses EGI Federated Cloud and PRACE resources and manages national and regional computing facilities ranging from clusters of multicore processors to cloud clusters. (See Table 1.2)

computing resources	Provider	EU	NA	RE	TRL	use cases
EGI Federated Cloud + Grid	EGI	X			9	All
CINECA	PRACE	X			9	All
CMAST	Italy	X			9	2,3,5
CRESCO	Italy	X			8	2,3,5
RECAS	Italy		X		9	2,3,5
ZIH	Germany		X		9	1,2,4
MoSGrid	Germany		X		9	3,4,5
UCM Computer cluster	Madrid			X	9	2,3,4
Computer Center. Nat. Inst. Chem	Ljubljana			X	8	8
Openstack cloud	Perugia			X	7	2,3,5
Linux cluster	Perugia			X	8	2,3,5
FLAVUS cluster	Tübingen			X	8	4

Table 1.2: Computing resources in the Sumo-Chem RI

CMAST is a **Virtual Laboratory** to support research in Chemistry. It uses extensively the computational resources and innovative on-line services of the EGI cloud and grid resources. It is also integrated with CRESCO that provides a unified user environment and a seamless user-friendly access method to combine computing resources and experimental facilities. **CRESCO** is a production grid of computational resources belonging to ENEA DTE-ICT. **ReCaS** incorporates compute resources of 4 national Italian data centres (Napoli, Bari, Catania, Cosenza) of the national Italian Grid Infrastructure (IGI) that is part of the European Grid Infrastructure (EGI) and INFN. The key users are the research institutions in southern Italy regions and CERN (ATLAS, CMS, ALICE, LHCb). **MoSGrid** is the compute infrastructure that provides Grid services for molecular simulations leveraging on an extensive use of D-Grid-Infrastructure for high-performance computing. MoSGrid handles metadata and their provision for data mining and knowledge generation. Via a portlet, researchers can access data repositories where information on molecular properties as well as on "recipes" - standard methods for the provided applications – are stored. Using these recipes simulation jobs can be automatically generated and submitted into the Grid. Moreover, the users are also supported at the analysis of their calculation results. Through the cross-referencing of different result data sets new insights can be achieved. The data repository additionally allows external referencing of simulation results.

Data resources. Researchers in Chemistry utilize a multitude of different data resources. They range from experimental data recorded in the own lab, over large infrastructure facilities to specific analysis and simulation applications. Currently all these resources are stored in their own data structures and formats. The need for a standardized annotation with metadata is immanent to facilitate the researcher's work, to improve interoperability and to enhance resilience. A uniform, open metadata format accompanied by robust ontologies will serve as cap stone for Sumo-Chem.

1.3.2 Sumo-Chem Concept

Currently, the Chemistry sub-domains have their own isolated "islands of research facilities and infrastructures". There are three consequences of this situation. First, researchers of one sub-domain either cannot access facilities of other sub-domains or it is too complicated to use them. Second, expensive research facilities might be underutilized. Last but not least they cannot properly share their knowledge, i.e. scientific data. The Sumo-Chem RI will create a "virtual continent" of these "islands" connecting them via a 3rd generation science gateway. Researchers as the citizens of this continent will use data as a common currency for communication among these "islands". There will be two-way communication

between Computational and Experimental Chemistry in this "continent". Researchers will run experiments and publish results using the Sumo-Chem RI. Analysing this data Computational Chemists will design simulations that can complement experiments to produce new research achievements. The same kind of cooperation will be supported from the other end, i.e. researchers will run simulations that results can be further checked in experiments. The "virtual continent" will incorporate 5 European, 4 national and 4 regional research facilities (See Table 1.1); and 4 European, 3 national and 5 regional computing resources (See Table 1.2); plus access to European, national and regional data archives, databases, data centres and data storages using either basic data transfer protocols or advanced B2xx services.

The **Sumo-Chem architecture**, presented in Figure 1, combines four key entities: research facilities, computing/data resources, science gateway and researchers.

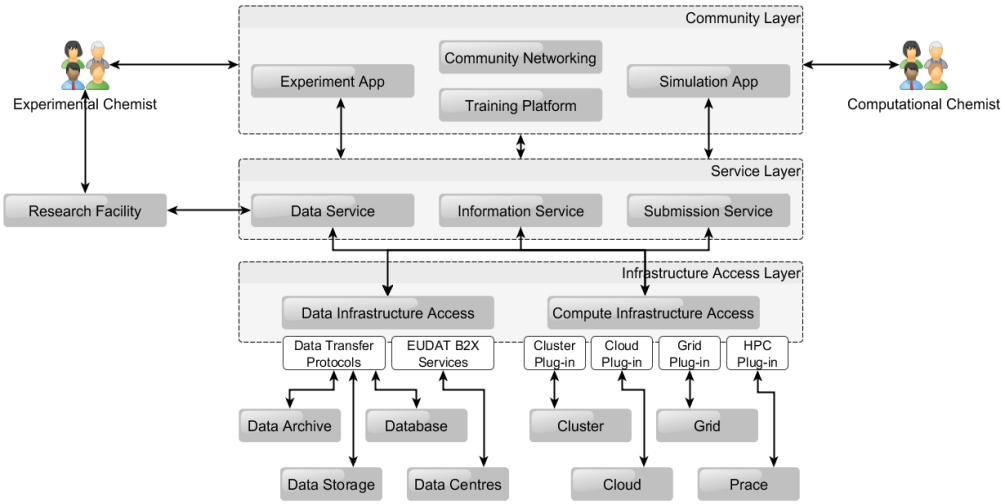

Figure 1: Sumo-Chem Architecture enabling convenient access for researches to the data and compute infrastructure.

The science gateway will enable researchers to access research facilities, computing and data resources. It will have three layers: community, service and infrastructure access layer. The community layer will offer social media type services allowing Experimental Chemists to run experiments on remotely available research facilities. This layer will provide to access the submission service to run simulations. It will also support training activities and community building. The service layer will connect researchers to the research facilities and e-infrastructure resources using microservices managed by a service orchestrator. The set of microservices will contain a data, information, monitoring, resource broker, submission, visualization, etc. service. Fig. 1 contains three of these services as an example. The major innovation will be the data service that will connect Experimental and Computational Chemists through scientific data. Experimental Chemists will use the data service to manage experimental data while Computational Chemists will run simulations through the submission service using the data service. The submission service will support running jobs, pipelines and workflows. The infrastructure access layer will have two services: computing and data infrastructure access service. The first one will manage access to major computing resources such as cloud, cluster, grid and supercomputer. The second one will manage data using different types of data resources, such as data archives, databases, data collections, data storages using EUDAT B2xx and MASi services, and major data transfer protocols.

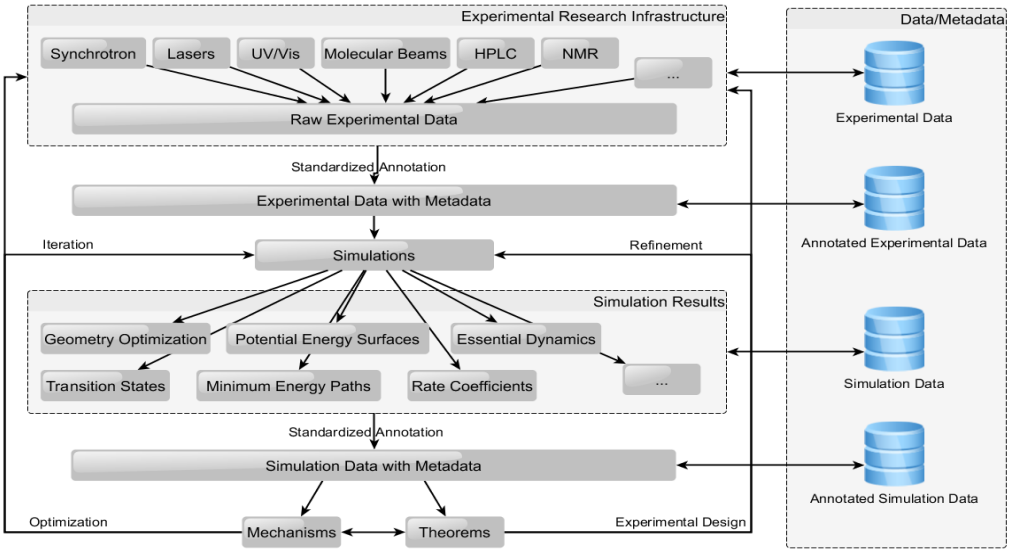

Figure 2: Data flows within the Sumo-Chem community

Data in Sumo-Chem. Data interoperability is a major technical challenge in the Sumo-Chem RI because data must enable cooperation inside and among sub-domains of Chemistry involving both Computational and Experimental

Chemists. In Chemistry the data-life-cycle ranges from primary experimental data over simulation results to fully annotated scientific data. We will develop a data management approach that will facilitates reusability and consequently reproducibility using metadata. Experimental researchers produce a large volume of primary data in many different data formats. These differences make it difficult to share data among researchers and harness it. Storing and sharing primary experimental data might not be meaningful because it does not contain information about how it was obtained and processed. Adding metadata to primary data, particularly provenance information supports sharing scientific data. Metadata can describe the method and the equipment used, measurement protocol applied, conditions and parameters specified, etc. This information enables researchers to evaluate the experiment itself and to decide further usage of data.

The same approach must be followed with simulated data as illustrated in Figure 2. Similarly to experimental data, significant efforts have been spent to describe computing resources needed, implementation methods used and scientific analysis applied in simulations. There are a few approaches that support the transparent storage and sharing of scientific simulation data. Markup languages like CML or its derivate MSML offer ontologies for the hierarchical representation of simulation protocols as workflows including relevant input and output data, as well as the analysis. QC-ML and consequently Q5Cost follow a similar tree representation overall focusing more on quantum chemical simulation data.

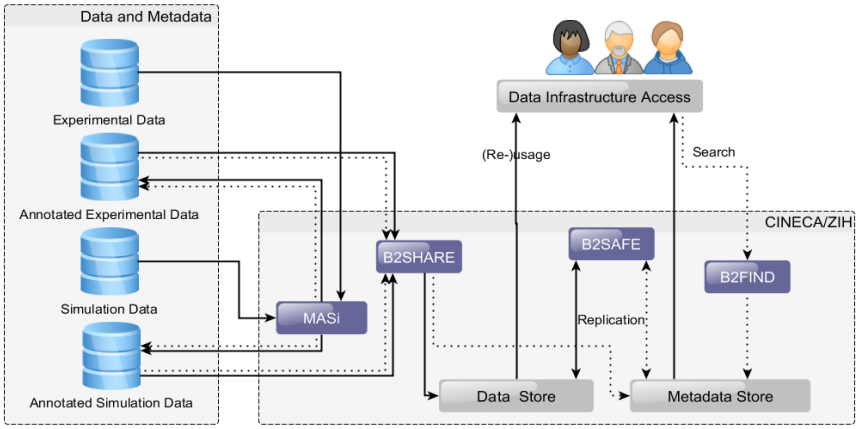

Figure 3: Sumo-Chem data management using EUDAT and MASi services for data ingestion, storage, replication and search (Remark: Data flows are indicated by bold lines, flow of metadata is shown as dashed line**).**

The proposal will build on the experience with MSML and Q5Cost to create a uniform standardized representation of the whole data life cycle ranging from initial experimental data to the analysis of simulation data. It is anticipated to feed the metadata to B2FIND making it available beyond the closer Computational Chemistry community. Special emphasis will be put into the storage of 'good' protocols, accepted in the field, on a meta level. By representation through an XML based markup language individual tasks along such community workflows are decoupled from actual implementations e.g., specific software packages while maintaining the actual purpose of the respective task. For example the geometry optimization of a given molecule can be accomplished with numerous tools, while the final conformation should be sufficiently comparable among all implementations. A meta description of such tasks supports the reproducibility and sustainability of scientific protocols in the best possible way.

The data will be hosted by CINECA and ZIH data centers employing a federated storage solution compliant with EUDAT approaches as depicted in Figure 3. Annotated primary data from experiments and simulations will be transferred via the MASi service uploading valuable content to the community data hub. The access to individual data sets will be handled via groups and access control lists allowing fine-grained control about what is shared with whom, which is especially important prior to scientific publication in compliance with existing scientific data policies of the facilities. The security of the data and metadata will be ensured through the usage of European AAI services utilizing federated identities (eduGAIN) wherever feasible. We will closely observe the results of the European AARC project and their goal to create an interdisciplinary AAI solution based on existing systems and evaluate its applicability within Sumo-Chem.

1.3.3 Approach and methodology.

Sumo-Chem will have two Joint Research Activities (**JRA**): WP1 and WP2; three Service Activities (**SA**): WP3, WP4 and WP5; one Network Activity (**NA**): WP6; and one Management Activity (MGT): WP7 work package. WP1 will develop and implement the Sumo-Chem architecture integrating the existing services and elaborating new services as microservices. WP2 will focus on data management for data creation, publishing, sharing, curation and preservation. It will pursue innovation to support data sharing using metadata, ontologies and provenance. Cooperation between WP1 and WP2 will deliver significant advances in how researchers can share data because of the substantial conceptual simplification and improvement in usability they will achieve. WP3 will produce the production releases of the science gateway considering requirements of each use case. This work package will deploy, configure and manage the science gateways for use cases. It will also provide technical support for use cases. WP4 will address societal challenges in climate while WP5 in energy through the relevant use cases running experiments and simulation on the Sumo-Chem RI. WP6 will organise and run dissemination and training events to promote technical understanding of the Sumo-Chem

RI, develop skills required to use this infrastructure, reach wider communities and provide an opportunity for multi-disciplinary research that will seed common solution strategies. The project activities will be coordinated by WP7 via the project's intranet, via regular physical and virtual project meetings. WP7 will also run the administrative and financial management tasks.

Technology Readiness Levels. The levels of research facilities and computing resources to be integrated in the Sumo-Chem RI are given in Table 1 and Table 2. The TRD values of simulation packages are in the range of TRL 6 and TRL 9. The project consortium will analyse each simulation package and will make recommendations for the Chemistry community which one to use considering their functionality and TRD value. The community layer of the science gateway will offer customized portlet apps while the service layer will be based on the gUSE framework. These frameworks TRL value starts from 6. The EUDAT B2xx and MASi services as well as the gUSE DCI Bridge of the infrastructure access layer has TRL value 7, 6 and 8 respectively. Considering these TRD values the major technical task of Sumo-Chem will be integration of research facilities and e-infrastructure resources into the RI and developing and/or upgrading services for example the Sumo-Chem Data Service.

1.3.4 National and international research linked to the project.

The Chemistry community will cooperate with a wide range of associations and organisations: COMPCHEM (EU Computational Chemistry VO), CMMST (EU Chemistry, Molecular and Materials Science and Technologies Virtual Research Community), CHEM.VO.IBERGRID (EGI-Inspire VO), MoSGrid and with EU and national research projects: DFG Priority Program 1740 (Reactive Bubbly Flows), EoCoE: (Energy Oriented Centre of Excellence), Multi-scalSOLAR COST project (multiscale simulations of materials for PV technologies) and KIC Raw Materials (European Network for critical raw materials). The science gateway will be built on open source frameworks and services mainly developed within European research projects such as EDGI, ER-flow, SHIWA and SCI-BUS while B2xx services were developed by EUDAT.

1.4 Ambition

Conceptual ambitions: The project will pioneer a new way of cooperation between Computational and Experimental Chemistry creating an RI that will focus on data management to support research cooperation. It will break down barriers isolating research groups clustered around particular research facilities and technologies providing access to wide range of facilities and technologies. The RI will be built on deep understanding of the ways in which this community uses data. The project will analyse why more researchers do not exploit the considerable potential of available research facilities and e-infrastructure resources to run sophisticated experiments and simulations. The project will identify what approaches work well, what limitations they encounter and what they need. The Sumo-Chem RI will also support multi-disciplinary research with the climate and energy community for addressing the complexities in societal challenges. This research cooperation will help pooling the intellectual efforts in creating and refining data management approaches, such as data preservation, identification and citation that can be used across multiple disciplines. **Technological ambitions.** The major technical challenge comes from the heterogeneity of the Chemistry community. Researchers use different types of research facilities to run experiments and different e-infrastructure resources to run simulations. They produce different types of data in different data formats. The RI must address this heterogeneity providing a user interface that seamlessly hides differences in data, e-infrastructure resources and research facilities. The key beyond the state-of the-art solutions will be a service orchestrator to manage a set of microservices to address this heterogeneity and the Sumo-Chem Data Service. The microservices will provide maintainable and sustainable services. This approach will enable creating small, well-defined building blocks of functionality whilst enabling a completely flexible and agile approach to front-end development. Partitioning functionality into microservices will enable agile addition of functionality and reduce the risk of complexity delaying response to scientific requirements. Researchers will communicate with the RI through a web-enabled interactive front-end in the community layer, called dashboard. It will be a social media type user interface that will provide researchers with a new means of understanding, thinking about and working on scientific processes represented as either experiments or simulations. The dashboard will allow interaction between researchers themselves to share data at one side and use research facilities and e-infrastructure resources at the other side. The Sumo-Chem service layer will contain a service orchestrator to manage microservices. These services will manage access to different types of research facilities, computing and data resources available in the RI. The Sumo-Chem Data Service will handle the whole data lifecycle including creating, publishing, sharing, curating and preserving data.

Innovation potential. The key innovation of the project will be the Sumo-Chem RI itself that will incorporate research facilities used in experiments and computing and data resources used to run simulations. This RI will enable two-way research cooperation between Experimental and Computational Chemistry through publishing and sharing data via the Sumo-Chem Data Service. At one side researchers can run simulations to verify experimental results and design further simulations based on these results. At the other side analysing simulation results researchers can plan more efficient experiments excluding theoretically non-sensitive options. Researchers will leverage on this two-way data exchange to follow new research challenges to create and validate improved or new materials that business, industry and society can use. The Sumo-Chem RI will enrich the Chemistry community with new competences and technological solutions to address the climate and energy societal challenge.

2. Impact

2.1 Expected impacts

Researchers access to RI. They will have wider, simplified, and more efficient access to European, national and regional facilities and resources to conduct their research irrespective of location where they are through the Sumo-Chem RI. This RI will be an open architecture that will serve as transparent basis for future scientific developments inside and outside Chemistry. This open architecture will enable connecting further research facilities and resources to extend the outreach of the RI outside the Sumo-Chem project consortium. As a result, researchers who are not involved in the project will be able to access and use this RI. To further improve research Sumo-Chem will develop a uniform and standardized data management to handle data ranging from experimental to simulation data. Moreover, the consistent annotation with provenance and metadata information ensures reusability and reproducibility of scientific results, improving trust into their reliability. This data management solution will allow sharing of information and knowledge between the Chemistry and other communities such as Climate and Energy community and between academia and industry.

Addressing societal challenges. The Chemistry community identified the Climate and Energy societal challenge focusing on energy efficiency, low-carbon energy and waste management. Each use case specified the relevant research issues. (See Table 1.3 – 1.5). The Sumo-Chem RI will be open to researchers of the Climate and Energy community to allow joint multi-disciplinary research.

use case 1	investigating energetic molecules of potential interest in energy storage/release
use case 6	developing more efficient, cleaner and fuel flexible combustion devices/processes for distributed energy production addressing requirements of the Energy Trilemma (security, equity and sustainability of energy production systems); reducing environmental and health impact of alternative and fossil combustion systems

Table 1.3: energy efficiency focus area

use case 2	studying the photochemistry and reactivity of energetic materials, the laser manipulation of materials, the dynamics, stereo-dynamics and quantum control of elementary chemical processes
use case 3	development of technological applications, related to CO_2 abatement (e.g. destruction in electric discharges or by molecular sieves), controlled thermonuclear fusion energy, efficient use of energy in technological applications, such as nuclear fusion by inertial confinement, material science for aerospace and microelectronics applications, plasma-based energy recovery devices
use case 4	development of metal complexes for solar devices, efficient energy transfer, determination of electron and energy transfer pathways
use case 5	promoting usage of renewable energies by improving storage of renewable energy as carbon neutral fuels
use case 7	designing new materials at the nanoscale by combining experimental and numerical results, to improve production of specialized nanomaterials for energy applications.
use case 8	improving production of biodiesel fuel and reducing the need for fossil fuels.

Table 1.4: Low-carbon energy focus area

use case 3	plasma modelling of applications related to waste treatments (plasma torches, syngas production)
use case 4	development of ecological and sustainable catalysts for production of biodegradable plastics from renewable resources to address depletion and exploding costs of fossil resources, climate change and growing landfill sites
use case 5	recycle CO_2 by reduction using H_2 to carbon compounds useful for syntheses as well as modelling of the related system based on an accurate prediction of rate coefficients and integration of kinetic equations
use case 6	exploitation of novel energetic molecules that derive from different and locally diverse sources to minimize the CO2 and pollutant emission

Table 1.5: Waste management focus area

Multi-disciplinary research and ESFRI cooperation. Addressing societal challenges requires multi-disciplinary research and cooperation with ESFRI projects. Use case 6 and use case 7 will coordinate joint research with the Energy community on energy efficiency (Table 1.3) and low-carbon energy (Table 1.4), respectively. Use case 4 will lead the cooperation (Table 1.5) with the Climate community. The use cases will also collaborate with the Physical Sciences community. Table 1.6 summarises the prospective cooperation with ESFRI projects.

field	ESFRI initiatives	use cases
Energy Sciences	ECCSEL	use cases 5, 6, 7, 8
Environmental Sciences	IAGIOS	use cases 5, 6
Physical Sciences	IFMIF, ELI, EuroFEL	use cases 1, 2, 3, 4

Table 1.6: Research cooperation with ESFRI initiatives

Research facilities and **e-infrastructure resources providers** are Sumo-Chem project partners. They will develop synergies and complementary capabilities, leading to improved and harmonised services by leveraging on the 8 Sumo-Chem use cases. This will avoid duplications of facilities and services and will lead to their improved use across Europe. Economies of scale and saving of resources are also realised due to common development and the optimisation of operations. The integration of major research facilities, e-infrastructure resources and of the community knowledge base (collections, archives, structured scientific information, data infrastructures, etc.) will lead to a better management of data collected or produced by these facilities and resources. The key **innovation** of the project will be the Sumo-Chem RI that will allow two-way research cooperation between Experimental and Computational Chemistry through

publishing and sharing data via the Sumo-Chem Data Service. Researchers will leverage on this two-way data exchange to follow new research challenges to create and validate improved or new materials that business, industry and society can use. The Sumo-Chem RI will target new competences and technological solutions to address the climate and energy societal challenge. The **main obstacles** are the standardization of data and the implementation of an effective collaborative environment. Master-up has already developed tools for the evaluation of the collaboration activities (GriF) and for the rewarding of best practices through credits (GcreS) that will be adopted by Sumo-Chem.

2.2 Measures to maximize impact

2.2.1. Dissemination and exploitation of results

The communication activities will be divided in internal (within the Sumo-Chem community) and external (with potential stakeholders). The **internal communication** will aim on reinforcing cooperation among the community to promote effective synergies. The key to accomplish this goal will be running communication channels among all parties: project partners, user communities, facility and resource providers. The main internal communication channel will be the project website and regular on-line project, work package and use case meetings. The project will also use traditional communication channels such as the ***ECTN newslette***r, published quarterly, the ***VIRT&L-COMM*** open access journal to present the RI and use case achievements. The **external communication** will focus on disseminating the Sumo-Chem success stories to potential new stakeholders, such as user communities, facility and resource providers, industry partners etc. to raise their awareness about the Sumo-Chem RI. This will be accomplished through demonstrations, presentations and publishing Sumo-Chem papers in scientific journals. Attending events will also play an important role in outreach activities to new stakeholders. To promote the Sumo-Chem RI and train its prospective users the project will elaborate a dissemination and training plan to be run in parallel with the usual activities of the project partners (courses, conferences, summer schools, training events, etc.). These activities will be focused also on multi-disciplinary research, technology transfer between academia and industry.

Dissemination events. The project will organise an annual Sumo-Chem workshop at the Computational Chemistry Conference to raise awareness of the Chemistry community about the Sumo-Chem RI involving facility and technology providers, research and SME partners. The project partners will also present the Sumo-Chem RI at other Chemistry conferences and EGI, EUDAT and PRACE events. They will outline the RI itself, how to use it (focusing on the synergetic activities supported by the RI), and how to extend it. Particular attention will be devoted to the data management highlighting how to use different data formats, how to use metadata and provenance. The project partners will present and demonstrate the use cases. The project partners will also approach researchers from inside and outside the Chemistry community to identify further prospective use cases to be ported to the RI. **Training events.** ECTN, Master-up and Polymechanon will organise a summer school in every project year on how to use the RI (involving research facilities and e-infrastructure resources providers) for junior researchers and PhD of the Theoretical Chemistry and Computational Modelling (TCCM) ITN JDP. ECTN will define specific Learning Objectives (LO) for each summer school using the GLOREP archives. ECTN's, Master-up's and Polymechanon's expertise will guarantee that not only researchers will benefit from training events but also PhD students and SME employees thanks to the use of multi-media technologies.

2.3 Measures to achieve the impacts

2.3.1 Data Management Plan

Sumo-Chem will deal with the whole-data-life-cycle from primary experimental data to annotated simulation data. Metadata annotation employing a standardized markup format and corresponding ontologies will enable Sumo-Chem to handle the plenitude of data and formats. A distributed storage infrastructure will host the data and make it available persistently to the community through the usage of EUDAT B2xx and MASi services. Data will be curated by the related use case as will be specified in an *ad hoc* agreement. Hence not only the data itself will be available for the scientific community but also the protocols used to generate it, largely improving reproducibility and reusability.

2.2.3 KPIs of communication activities

The project will run specific activity to disseminate and exploit project's results. The involvement of SMEs and since long active associations will allow to put on a solid ground such aspect by setting-up the strategies to guarantee the maximum impact and sustainability beyond the project lifetime. Moreover, the requirements coming from the project partners will be regularly collected and analysed by the project technical management to ensure that the requirements are adequately prioritized in the development technical plans, thus maximizing the interoperability with the existing e-infrastructures. Besides the technical effort to streamline the adoption of the RI products by other communities a sustainable exploitation of the outcomes is only assured if the research communities uses them. Any networking strategy addressed to expanding the user base of the RI products among research communities and private companies needs to take into consideration the organizational possibilities and constrains of the research sector. The Consortium here counts on the strong support of the different and well established research institutions plus, as well, of a pool of SMEs which will act as conduit of the new services towards those communities outside the project initiative.

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