OPEN FORCE FIELD CONSORTIUM

Daniel Crawford, The Molecular Sciences Software Institute, Blacksburg, VA 24060

Today, the Molecular Software Sciences Institute launches **The Open Force Field Consortium ("OpenFF Consortium")** an academic-industry collaboration designed to improve computer models used to guide pharmaceutical drug discovery.

This effort, which was spearheaded by scientists from the University of California Irvine, Bayer, and GSK, focuses on improving the energy models, or force fields, used extensively in computer-aided drug design. Modeling tools based on force fields assist the development of therapeutics for diseases such as cancer and neurodegenerative disease throughout academia and industry. However, accuracy falls short of the mark in many cases. The OpenFF Consortium focuses on changing that through automated development and improvement of new force fields, facilitating rapid increases in accuracy.

This consortium brings together researchers from across academia and industry to create an entirely open force field platform. All software, force fields, and development tools will be fully open source and available to everyone, as the participating organizations recognize that this infrastructure can and should help the entire field.

The Consortium focuses on the development of an extensible, open source toolkit for constructing, applying, and evaluating force fields; the curation of public datasets necessary to build high-accuracy biomolecular force fields; and the generation of improved biomolecular force fields. Academic and industry partners work together help the initiative succeed.

Consortium partners, both academic and commercial, bring a great deal of expertise to the initiative. The governing board consists of five initial Principal Investigators and two elected industry representatives from the advisory board. Thus, industry partners give key scientific input and involved in steering the Consortium.

Commercial partners provide the primary support by means of financial and in-kind contributions for the work. Initial partners include BASF; Bayer; Boehringer Ingelheim; Vertex Pharmaceuticals; Merck KGaA, Darmstadt Germany; XtalPi; and F. Hoffman-La Roche Ltd.,The MolSSI serves as a coordinating intermediary, and helps to ensure developed software follows best practices as and encourages synergy with other open-source efforts within the molecular sciences.

"We aim to democratize the construction of accurate molecular mechanics. This effort will build a community around an open, modern, statistically-grounded set of software tools allowing users to build molecular mechanics force fields from their own selected physical property and quantum chemical datasets. This same infrastructure will allow us to produce better force fields, as well," said Michael Shirts (University of Colorado Boulder).

"Force fields represent the foundation of molecular simulations and modeling — a real community resource. Everyone uses them, but improving them is an often unglamorous task. We're very excited that our industry partners recognize the importance of this problem and have joined us to help support this important initiative, so that we can improve modeling as a whole,"

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said David L. Mobley (UC Irvine).

The MolSSI at Virginia Tech is funded by the NSF and serves as a coordinating intermediary, helping to ensure that the developed software is broadly useful and sustainable. "The MolSSI is proud to facilitate the industrial-academic connections represented by the Open Force Field Consortium," said T. Daniel Crawford, director of The MolSSI. "This falls squarely within our mandate to provide the global computational molecular sciences community the tools it needs t*o explore larger and more complex scientific challenges than ever before."*

For more information about the **Open Force Field Consortium,** visit http://openforcefield.org. OpenFF is also seeking potential additional funding from foundations and federal agencies, and welcomes additional commercial partners interested in joining in support of the initiative. For more information about the MolSSI, visit http://molssi.org.

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