

# From RDKit to MD simulation in seconds: An introduction to Open Force Field

Jeff Wagner, OpenFF Technical Lead



### The Open Force Field Consortium

#### **INDUSTRY**

AbbVie OpenEye

Amgen Pfizer

AstraZeneca Redesign

Bayer Roche

Cresset Ventus

Eli Lilly Vertex

Janssen ... and others



Open Molecular Software Foundation



### **ACADEMIC**

2

John Chodera (MSKCC)



Michael Gilson (UC San Diego)



David Mobley (UC Irvine)



Michael Shirts (CU Boulder)

### **PROJECT STAFF**



Jeff Wagner Technical Lead



Lily Wang Science Lead

### Plus affiliates:

- Danny Cole (Newcastle)
- Lee-Ping Wang (UCD)
- Dennis Della Corte (BYU)
- MolSSI (Virginia Tech)

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Open source **Python Toolkit**: use the parameters in most simulation packages

Open curated QM / physical property datasets: build your own force fields



Open infrastructure: Run your own benchmarks; fit your own FFs

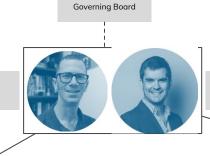


**Open science:** Everything done in the open/everyone can get involved

### **Org chart** Governing Board David Mobley James Eastwood Acting PM Acting PM Lily Wang Science Lead Jeff Wagner Technical Lead Alexandra McIsaac Brent Westbrook Matt Thompson Joshua Mitchell David Dotson Staff scientist Staff scientist Software scientist Sci. Comm. Software scientist

# **Org chart**









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Science Lead

Tobias Hufner OpenFF Alumnus



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Matt Thompson Software scientist

Jeff Wagner Technical Lead



Joshua Mitchell Sci. Comm.



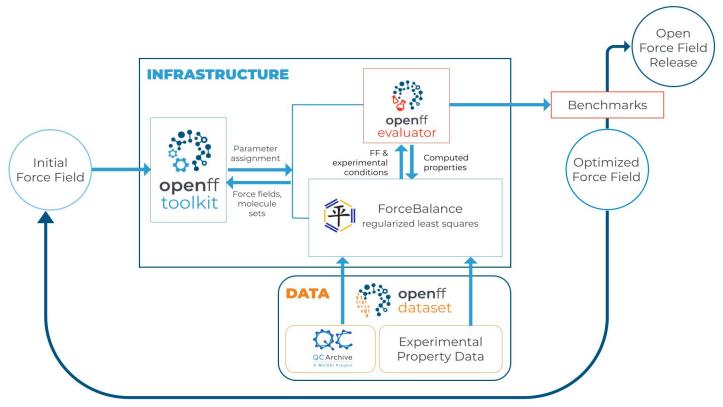
Meghan Osato Mobley PhD



David Dotson Software scientist

### We create new force fields and systematically improve

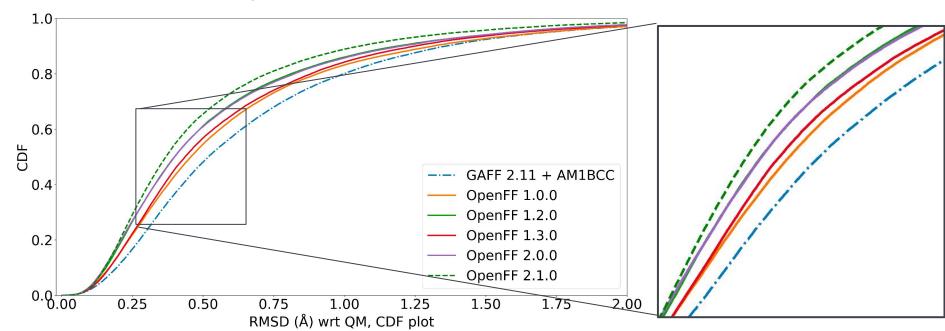




## OpenFF already makes one of the best modern public small molecule force fields

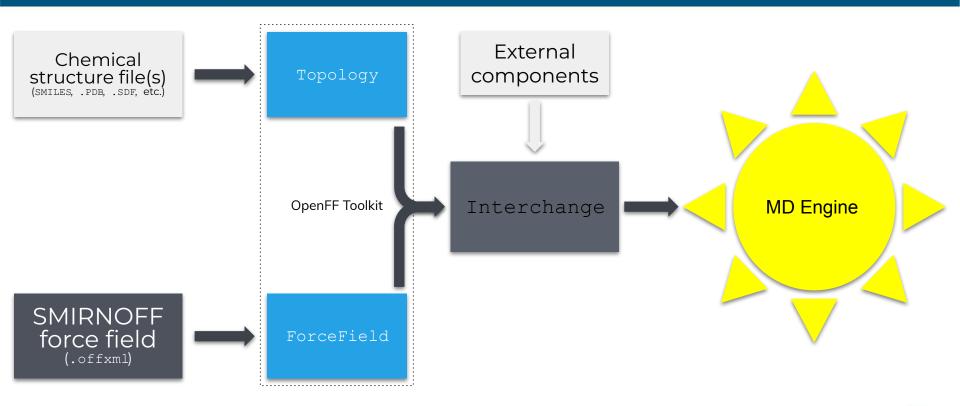






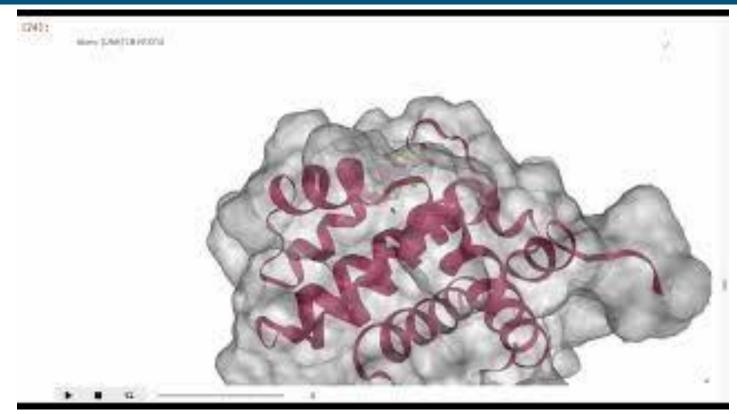
### The OpenFF Workflow





### And now, for something completely different...







### **Acknowledgments**



- Greg and the RDKit community
- All our partners, past and present (see openforcefield.org)
- Our team and alumni
- The OpenFF Initiative and community
- Virginia Tech for initial hosting
- OMSF for current hosting
- OpenFE for collaboration, and testing
- The AMBER community and AMBER-family force fields (OpenFF began as a sibling)



### Get started at docs.openforcefield.org!

