An Online Database for TraPPE Force Field Parameters

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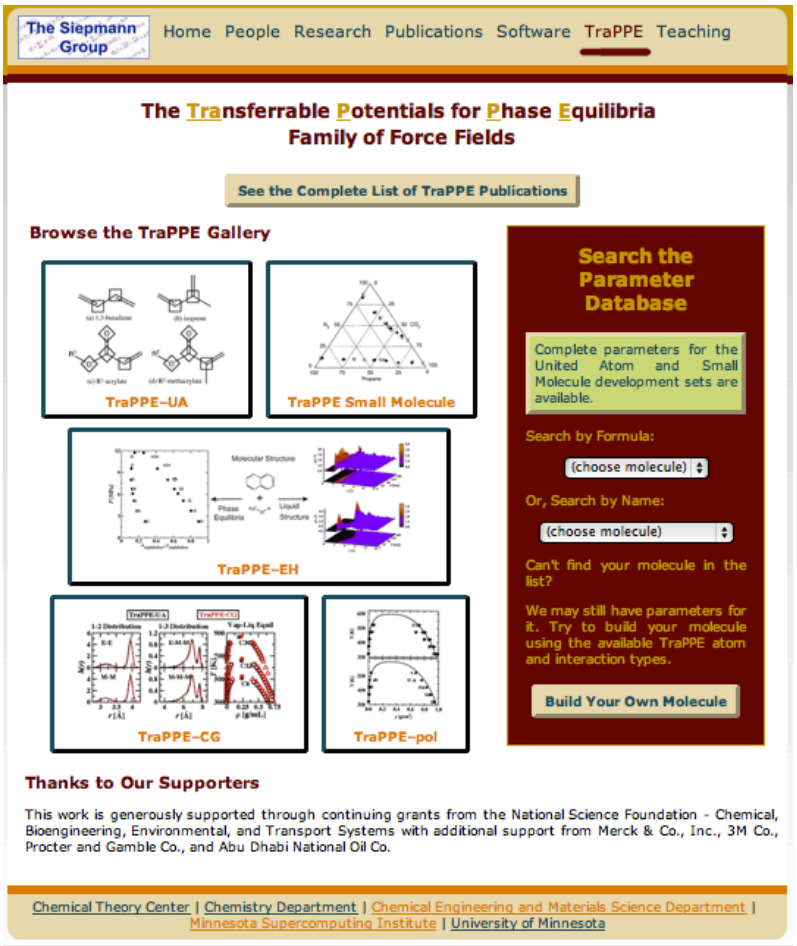
The Transferable Potentials for Phase Equilibria Force Field (TraPPE) is used to describe interactions between molecules of interest in molecular mechanics simulations. The TraPPE force field aims to be accurate, computationally efficient, and applicable to a wide range of chemical compounds, state points and thermophysical properties. To date, the TraPPE force field spans most of the common functionalities of small organic molecules and includes united-atom, explicit hydrogen, polarizable, and most recently, coarse-grain versions.



When new users wish to implement TraPPE models into their chosen simulation program, they face potentially prohibitive barriers to success: the TraPPE models are dispersed over dozens of separate publications and misinterpretations of the primary literature are common; the TraPPE force field makes specific choices for standard conventions that may require non-trivial code modifications for some simulation software. Therefore, an important goal for TraPPE developers is to encourage its broad use and accessibility. We present here the continuing development of a resource website and online searchable parameter database designed to provide new and experienced users with tools for successful implementation and validation of TraPPE. This work is done in collaboration with the Siepmann Group at the University of Minnesota.

http://www.chem.umn.edu/groups/siepmann/trappe/