Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Accurate predictions of biomolecular interactions using density functional theory based semi-empirical alchemical derivatives in chemical compound space ANATOLE VON LILIENFELD, Argonne National Laboratory — A small but relevant sub-set of chemical compound space is explored in terms of biomolecular interaction energies, and using analytical derivatives. When transmutating any two iso-electronic ligands their intermolecular energies are not necessarily monotonic functions, consequently the corresponding Hellmann-Feynman derivatives can fail to predict the right trends. Semi-empirical corrections, effectively linearizing the intermolecular energy in the interpolation parameter, promise to drastically improve the predictive power of these first order derivatives. For various biomolecules, including ellipticine interacting with DNA, we show that these semi-empirical derivatives yield predictions superior to alternative prediction schemes that are additive and derivative-free. As such, new evidence is presented in support of the conclusion that quantitative estimates of relevant properties of new molecules can be made without additional self-consistency calculations.

Anatole von Lilienfeld
Argonne National Laboratory

Date submitted: 10 Nov 2011 Electronic form version 1.4