

Abstract Submitted
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Accurate *ab initio* energy gradients in chemical compound space¹

ANATOLE VON LILIENFELD, Sandia National Laboratories — The design of chemical compounds with specific physical, chemical, or biological properties is a central goal of many fundamental as well as industrially relevant research fields. Analytical gradients in chemical space promise significant speedup in predicting properties of compounds without need to visit them. I will present analytical potential energy difference derivatives, based on the Hellmann-Feynman theorem, for any pair of iso-electronic compounds. The energies not being a monotonic function between compounds, these derivatives are insufficient to predict the right trends. Quantitative estimates can be made when the Hellmann-Feynman derivative is multiplied with a linearization coefficient that is defined for a reference pair of compounds. The results suggest that accurate predictions can be made regarding any molecule's energetic properties as long as energies and gradients of three other molecules have been provided. The linearization coefficient can be interpreted as a quantitative measure of chemical similarity. Presented numerical evidence includes predictions of electronic eigenvalues of saturated and aromatic molecular hydrocarbons. See J. Chem. Phys. 131 164102 (2009).

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