

Abstract Submitted  
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**Fast and Accurate Modeling of Molecular Energies with Machine Learning** ANATOLE VON LILIENFELD, Argonne National Laboratory, MATTHIAS RUPP, Technical University Berlin, ALEXANDRE TKATCHENKO, Fritz-Haber Institute Berlin, KLAUS-ROBERT MUELLER, Technical University Berlin — A machine learning model for the prediction of atomization energies of a diverse set of organic molecules, based on nuclear charges and atomic positions only, will be discussed. The problem of obtaining molecular energies across chemical compound space, aka. as solving Schroedinger's equation, is mapped onto a non-linear statistical regression problem of reduced complexity. We use eigenvalues of a "Coulomb"-matrix to encode all Cartesian and atomic number variables of a molecule. Regression models are trained on, and compared to, atomization energies computed with hybrid density-functional theory for a sub-set of the GDB-13 database consisting of more than seven thousand molecules. Cross-validation yields a mean absolute error of less roughly 10 kcal/mol. Applicability and transferability is demonstrated for the prediction of potential energy curves of unseen molecules.

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