

Abstract Submitted
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Molecular grand-canonical ensemble density functional theory O. ANATOLE VON LILIENFELD, MARK E. TUCKERMAN, New York University — The fundamental challenge of compound design, *i.e.* the reverse engineering of stable chemical compounds with predefined specific properties, originates in the high-dimensional and combinatorial nature of the *chemical* space [1] which is spanned by the grand-canonical variables (superimposed particle densities of electrons and nuclei). A rigorous description of chemical space, using a grand-canonical multi-component density functional theory framework, will be presented [2]. Specifically, a total energy density functional for molecular systems in contact with an electron and a proton bath is introduced using Lagrange multipliers which correspond to the energetic response to changes of the elementary particle densities. Results will be shown for a molecular Fukui function, for finite temperature estimates of the redox potential of ammonia, and for alchemical variation of the intermolecular energy of formic acid interacting non-covalently with 10 proton systems [2,3]. Implications for rational compound design [4] and multi-scale modeling shall be discussed.

[1] P Kirkpatrick, C Ellis *Nature* **432** 823 (2004)

[2] OAvL, M E Tuckerman *J Chem Phys* **125** 154104 (2006)

[3] OAvL, M E Tuckerman *submitted*

[4] OAvL, R Lins, U Rothlisberger *Phys Rev Lett* **95** 153002 (2005)

O. Anatole von Lilienfeld
New York University

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