Abstract Submitted
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From grand-canonical density functional theory towards rational compound design ANATOLE VON LILIENFELD, Sandia National Laboratories — The fundamental challenge of rational compound design, ie the reverse engineering of chemical compounds with predefined specific properties, originates in the high-dimensional combinatorial nature of chemical space. Chemical space is the hyper-space of a given set of molecular observables that is spanned by the grand-canonical variables (particle densities of electrons and nuclei) which define chemical composition. A brief but rigorous description of chemical space within the molecular grand-canonical ensemble multi-component density functional theory framework will be given [1]. Numerical results will be presented for intermolecular energies as a continuous function of alchemical variations within a neutral and isoelectronic 10 proton system, including CH_4, NH_3, H_2O, and HF, interacting with formic acid [2]. Furthermore, engineering the Fermi level through alchemical generation of boron-nitrogen doped mutants of benzene shall be discussed [3].
[1] von Lilienfeld and Tuckerman *JCP* **125** 154104 (2006)
[2] von Lilienfeld and Tuckerman *JCTC* **3** 1083 (2007)
[3] Marcon et al. *JCP* **127** 064305 (2007)

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