Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

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 engi-
neering 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 molecu-
lar 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$_2$O, 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].