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Towards computational materials design from first principles using alchemical changes and derivatives

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The design of new materials with specific physical, chemical, or biological properties is a central goal of much research in materials and medicinal sciences. Except for the simplest and most restricted cases brute-force computational screening of all possible compounds for interesting properties is beyond any current capacity due to the combinatorial nature of chemical compound space (set of stoichiometries and configurations).

Consequently, when it comes to computationally optimizing more complex systems, reliable optimization algorithms must not only trade-off sufficient accuracy and computational speed of the models involved, they must also aim for rapid convergence in terms of number of compounds ``visited''.

I will give an overview on recent progress on alchemical first principles paths and gradients in compound space that appear to be promising ingredients for more efficient property optimizations. Specifically, based on molecular grand canonical density functional theory [1] an approach will be presented for the construction of high-dimensional yet analytical property gradients in chemical compound space [2].

Thereafter, applications to molecular HOMO eigenvalues [3], catalyst design [4], and other problems and systems shall be discussed [5].

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[3] "Tuning electronic eigenvalues of benzene via doping", Valentina Marcon, O Anatole von Lilienfeld, Denis Andrienko, J. Chem. Phys 127 064305 (2007).
[4] "Alchemical derivatives of reaction energetics", Daniel Sheppard, Graeme Henkelman, O Anatole von Lilienfeld, J. Chem. Phys. in press (2010).
[5] O Anatole von Lilienfeld et al. in preparation (2010).