Abstract Submitted
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Fast and accurate covalent bond predictions using perturbation theory in chemical space KUANG-YU CHANG, ANATOLE VON LILIENFELD, University of Basel — I will discuss the predictive accuracy of perturbation theory based estimates of changes in covalent bonding due to linear alchemical interpolations among systems of different chemical composition. We have investigated single, double, and triple bonds occurring in small sets of iso-valence-electronic molecular species with elements drawn from second to fourth rows in the p-block of the periodic table. Numerical evidence suggests that first order estimates of covalent bonding potentials can achieve chemical accuracy (within 1 kcal/mol) if the alchemical interpolation is vertical (fixed geometry) among chemical elements from third and fourth row of the periodic table[1]. When applied to nonbonded systems of molecular dimers or solids such as III-V semiconductors, alanates, alkali halides, and transition metals, similar observations hold, enabling rapid predictions of van der Waals energies, defect energies, band-structures, crystal structures, and lattice constants [2].

[1] K. Y. S. Chang *et al* J. Chem. Phys. (2016)
[2] K. Y. S. Chang, O. A. von Lilienfeld, in preparation (2017); M. to Baben *et al* J. Chem. Phys. (2016); A. Solovyeva, O. A. von Lilienfeld Phys. Chem. Chem. Phys. (2016)

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