Exploration of Chemical Space for Designing Functional Molecules Accounting for Geometric Stability

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The design of functional molecules is regarded as searching for molecules with desired functionalities in chemical space populated by candidate molecules. Considering the geometric stability of molecules during the search process is crucial for designing realistic molecules. Here, we propose a method for designing functional molecules by exploring chemical space while explicitly accounting for geometric stability based on computational quantum alchemy.[1,2] The proposed design method allows the simultaneous prediction of functional molecule in the equilibrium geometry and its target desired property in an inverse design fashion, without preparing the molecular geometries and performing brute-force screening. The present design uses alchemical perturbation density functional theory (APDFT)[3] as the quantum alchemy to efficiently compute properties from iso-geometric molecular structures during the design process. The applicability of the design method is proven by obtaining molecules with desired atomization energy, electric dipole strength, and electronic energy in various chemical spaces: (BF, CO), (N_2, CO), (CH_4, NH_3), 18 BN-doped benzene derivatives, and 3.1×10^5 BN-doped phenanthrene derivatives. The proposed approach offers the basis for computational design of realistic functional molecules accounting for geometrical stability, going beyond the design of toy models and well-defined structures.

[1] T. Shiraogawa, J. Hasegawa, *J. Phys. Chem. Lett.* **13**, 8620–8627 (2022).
[2] T. Shiraogawa, J. Hasegawa, to be submitted.
[3] G. F. von Rudorff, O. A. von Lilienfeld, *Phys. Rev. Res.* **2**, 023220 (2020).