Alchemical normal modes unify chemical space

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In silico design of new molecules and materials with desirable quantum properties by high-throughput screening is a major challenge due to the high dimensionality of chemical space. To facilitate its navigation, we present a unification of coordinate and composition space in terms of alchemical normal modes (ANMs) which result from second order perturbation theory. ANMs assume a predominantly smooth nature of chemical space and form a basis in which new compounds can be expanded and identified. We showcase the use of ANMs for the energetics of the iso-electronic series of diatomics with 14 electrons, BN doped benzene derivatives (C 6 − 2 x (BN) x H 6 with x = 0 , 1 , 2 , 3), predictions for over 1.8 million BN doped coronene derivatives, and genetic energy optimizations in the entire BN doped coronene space. Using Ge lattice scans as reference, the applicability ANMs across the periodic table is demonstrated for III-V and IV-IV-semiconductors Si, Sn, SiGe, SnGe, SiSn, as well as AlP, AlAs, AlSb, GaP, GaAs, GaSb, InP, InAs, and InSb. Analysis of our results indicates simple qualitative structure property rules for estimating energetic rankings among isomers. Useful quantitative estimates can also be obtained when few atoms are changed to neighboring or lower lying elements in the periodic table. The quality of the predictions often increases with the symmetry of system chosen as reference due to cancellation of odd order terms. Rooted in perturbation theory the ANM approach promises to generally enable unbiased compound exploration campaigns at reduced computational cost.

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