Tata Institute of Fundamental Research
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Internal Webinar

Troubleshooting unstable molecules in chemical space

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A key challenge in automated chemical compound space explorations is ensuring veracity in minimum energy geometries—to preserve intended bonding connectivities. We discuss an iterative high-throughput workflow for connectivity preserving geometry optimizations exploiting the nearness between quantum mechanical models. The methodology is benchmarked on the QM9 dataset comprising DFT-level properties of 133,885 small molecules, wherein 3054 have questionable geometric stability. Of these, we successfully troubleshoot 2988 molecules while maintaining a bijective mapping with the Lewis formulae. Our workflow, based on DFT and post-DFT methods, identifies 66 molecules as unstable; 52 contain –NNO–, and the rest are strained due to pyramidal sp^2C. In the curated dataset, we inspect molecules with long C–C bonds and identify ultralong candidates ($r>1.70$ Å) supported by topological analysis of electron density. The proposed strategy can aid in minimizing unintended structural rearrangements during quantum chemistry big data generation.

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