# THE PRINCIPLE OF MOLECULAR RIGIDITY

VITALIY KURLIN

Understanding structure-property relationships for molecules requires a mathematical definition of a molecular structure. Any molecule keeps its functional properties under rigid motion (a composition of translations) within the same ambient environment. However, flexible deformations affecting the rigid shape can also change molecular properties. Hence the strongest equivalence between molecules in practice is rigid motion, which is a composition of translations and rotations. Then a molecular structure can be mathematically defined as the class of all atomic sets that can be exactly matched with each other by rigid motion. Since molecules often consist of indistinguishable atoms, the resulting problem is to design a complete invariant of unordered points under rigid motion with Lipschitz continuous distance metrics, all computable in polynomial time of the number of points, for a fixed dimension. It was a big embarrassment that, after the classification of triangles was known since ancient times, even the case of four unordered points in the plane had no better than a brute force solution involving exponentially many permutations of given points. The talk will present a recent extension of polynomial-time invariants [1], which satisfy the harder condition of realisability providing a continuous parametrisation of the moduli space of rigid clouds like geographic-style map of Earth. The experiments on the world's largest 3D molecular databases QM9 (130K+ entries) and GEOM (37M+ entries) confirmed the Principle of Molecular Rigidity saying that any real molecule is uniquely determined by precise enough geometry of only atomic centres.

[1] D.Widdowson, V.Kurlin. Recognizing rigid patterns of unlabeled point clouds by complete and continuous isometry invariants with no false negatives and no false positives. Proceedings of CVPR 2023 (Computer Vision and Pattern Recognition), p.1275-1284.