

Abstract Submitted
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Topological reaction coordinates to explore the structure of atomic clusters and organic molecule isomers from first principles FABIO PIETRUCCI, CECAM EPF Lausanne (CH), WANDA ANDREONI, CECAM and Institut de Théorie des Phénomènes Physique EPF Lausanne (CH) — We introduce a simple reaction coordinate based on spectral graph theory which describes the topology of the network of chemical bonds around a given atom. We employ the reaction coordinate in combination with DFT-based first-principles metadynamics to systematically explore the possible structures of silicon and carbon clusters (including fullerene-like cages) for sizes of tens of atoms. From our extensive exploration we are able to estimate the fractal dimension of the configuration space, which both for silicon and carbon clusters turns out to be quite low. Using the same approach we simulate the interconversion among a large number of chemically relevant organic molecules which are isomers of the C_4H_5N formula unit, and we demonstrate the possibility of automatically exploring isomerisation, association, and decomposition reactions without prior knowledge of the products involved.

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