Graph theory meets ab-initio molecular dynamics: atomic structures and transformations at the nanoscale

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We introduce a set of coordinates which describe the topology of the network of bonds among atoms. These coordinates are obtained from the contact matrix, they are invariant under permutation of identical atoms, and provide a clear signature of the transition between ordered and disordered structures. In combination with first-principles molecular dynamics and metadynamics, the topological coordinates are employed to explore low-energy structures of silicon clusters and organic molecules, demonstrating the possibility of automatically simulating isomerization, association, and decomposition reactions without prior knowledge of the products or mechanisms involved.

Finally we discuss the application of this new approach to the simulation of carbon nanostructures: we obtain transformation pathways for the reconstruction of zig-zag edges of graphene ribbons to 5-7 rings, as well as the folding of graphene into fullerene-like cages. Our results show that it is now feasible the blind exploration of complex structural rearrangements of nanostructures at finite temperature and at density-functional theory level of accuracy.

[1] F. Pietrucci and W. Andreoni, Phys. Rev. Lett. 107 (2011) 085504.