Simulating the structural diversity of astrophysical carbon clusters

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From a few atoms to bulk matter, carbon clusters show a significant ability to hybridize in sp, sp^2 or sp^3 chemical bonds, reflecting at finite size the wide allotropy of bulk carbon matter. In the interstellar medium (ISM), only the smallest molecules C_2 and C_3 and the fullerenes C_{60} and C_{70} have been observed so far [1,2]. The detection of C_{60} in Space was made possible from its peculiar spectral features originating from the high (icosahedral) symmetry that gives rise to only four infrared active bands. In order to obtain a better understanding of the formation mechanism of cosmic fullerenes and to identify other possible forms of carbon clusters in the ISM, it is essential to characterize the possible structural diversity of carbon clusters and map these structures onto their spectroscopic signature.

During this presentation, I will show an application of the software LAMMPS to simulate the structural diversity of carbon clusters. A few realistic potentials are available for carbon, which correctly account for bond breaking and formation and the various hybridization environments displayed by carbon. Here we have performed simulations using the reactive empirical bond-order potential (REBO) from Brenner [3] and the adaptive intermolecular reactive empirical bond-order potential (AIREBO) of Stuart and coworkers [4]. In order to obtain a database of structures we have performed Replica Exchange Molecular Dynamics (REMD) over a wide range of temperatures followed by quenching to identify local minima. The carbon cluster are then analyzed using global and local structural parameters.

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