Formation of endohedral fullerenes in atom-fullerene collisions

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Energetic ions or atoms colliding with aggregates of matter, such as molecules or clusters, can lead to exotic bond-forming reactions on very fast (sub-picosecond) timescales [1]. An important mechanism in these events is the knockout of one or more atoms, where individual atoms are permanently displaced from molecules when momentum is deposited through elastic scattering in the collision [1], a process that dominates at collision energies typically found in many astronomical environments.

Recently, we have performed a series of experiments where we collided fullerene anions with helium gas targets at center-of-mass energies below 100 eV. From these measurements we have determined a semi-empirical threshold displacement energy for the removal of individual carbon atoms from a C_{60} molecule/ion of 24.1 ± 0.5 eV [2], which is close to the value found for graphene and Polycyclic Aromatic Hydrocarbon (PAH) molecules [3,4]. We also observe the formation of endohedral He@ C_{60} fullerenes and defective fullerenes that still are capable of encapsulating He atoms, e.g. He@ C_{59} [2].

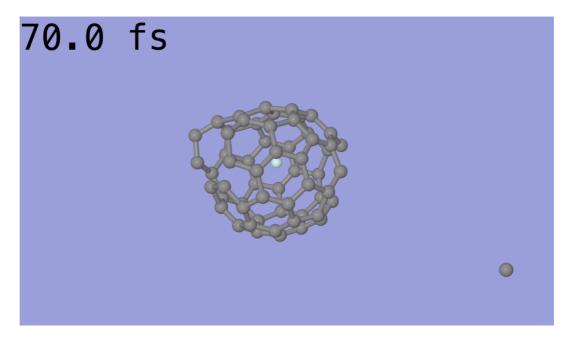


Figure 1: Snapshot from a classical molecular dynamics simulation of the formation of He@C59 in the collision between He and C_{60} at 80 eV center-of-mass energy.

References

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