

# Formation dynamics of dumbbell fullerene dimers $C_{118}$ , $C_{119}$ and $C_{120}$ upon collisions between $\alpha$ particle projectile and clusters of $C_{60}$ molecules

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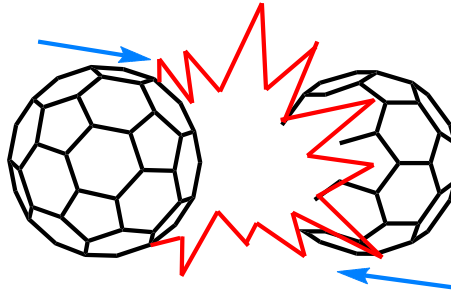
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Dumbbell-shaped fullerene dimers  $C_{118}$  and  $C_{119}$  have been recently produced through covalent bond formations upon the collisions between keV  $\alpha$  particles and clusters of  $C_{60}$  fullerenes [1, 2]. To unveil the formation mechanism and the characteristics of these mysterious fullerene dimers, we have carried out a systematic theoretical investigation which will be summarized in this talk.



Basically, a large number of systematic molecular dynamics (MD) simulations based on the self-consistent charge density functional tight-binding (SCC-DFTB) method [3] have been performed for the  $C_n^+ + C_{60}$  ( $n = 58, 59, 60$ ) collisions with various impact kinetic energies. The classical MD simulations using the Tersoff potential have also been carried out for comparison. The reliabilities of these methods have been carefully checked by comparing the step-by-step potential energies with the more sophisticated B3LYP/6-31G(d) DFT computations.

These MD simulations and the dissociation energy and barrier calculations will answer the following questions. Can a covalently-bonded fullerene dimer  $C_n$  ( $n = 118, 119, 120$ ) be formed and then survive in the experimental conditions (within a time scale of tens of microseconds and at rather low impact kinetic energy of a few eV)? What do these fullerene dimers, especially the odd-numbered dimer  $C_{119}$ , look like?

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- [1] H. Zettergren, P. Rousseau, Y. Wang, F. Seitz, T. Chen, M. Gatchell, J. D. Alexander, M. H. Stockett, J. Rangama, J. Y. Chesnel, et al., *Phys. Rev. Lett.* **110**, 185501 (2013).
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  - [3] M. Elstner, D. Porezag, G. Jungnickel, J. Elsner, M. Haugk, T. Frauenheim, S. Suhai, , and G. Seifert., *Phys. Rev. B* **58**, 7260 (1998).