Materials Science

MOLECULAR DYNAMICS COMPUTER SIMULATIONS OF NOBLE GAS DISC / C_{60} FULLERENE COMPLEXES

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We present the results of Molecular Dynamics computer simulations of noble gas discs placed around a central C_{60} fullerene molecule. Two aspects of disintegration of the system are explored: thermal and mechanical. In the former scenario the system melts, exhibiting diffusion between the lobes and finally the system disintegrates. In the latter case rotation causes the adsorbed layer to flatten into a single ring, which orbits the fullerene in a choppy fashion at low angular momentum values. As rotation increases the ring responds by orbiting in a smoother fashion; in addition smaller lobes are produced farther away from the central fullerene. Results are compared across several noble gas species.