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Carbon nanotube – metal cluster bond strengths: implications for catalytic growth. PETER LARSSON, Condensed Matter Theory Group, Physics Department, Uppsala University, Box 530, SE-751 21, Uppsala, Sweden, FENG DING, Rice University, ME & MS Department, Houston, TX 77005, J. ANDREAS LARSSON, Tyndall National Institute, Lee Maltings, Prospect Row, Cork, Ireland, ARNE ROSEN, Physics Department, Goteborg University, SE-412 96, Goteborg, Sweden, RAJEEV AHUJA, Condensed Matter Theory Group, Physics Department, Uppsala University, Box 530, SE-751 21, Uppsala, Sweden, KIM BOLTON, Physics Department, Goteborg University, SE-412 96, Goteborg, Sweden — Catalysts play a crucial role in the production of carbon nanotubes (CNTs). Although a lot of experimental effort has been devoted to finding metals and alloys to optimize CNT growth, the importance of the CNT-metal interactions at the microscopic level are not well understood. Previous simulations based on analytic force fields indicate that a critical role of the catalyst particle is to maintain an open end of the growing CNT, and that sufficiently strong CNT-metal bond strengths are required for this criterion to be met. Here we report CNT-metal bond strengths obtained from density functional theory for a variety of metal clusters. In agreement with the simulations, these calculations reveal that CNT interactions with metals used for production (e.g., Fe and Ni) are stronger than for other metals (e.g. Au). These bond strengths are also compared to the C-C bond energies that form when a cap forms at the end of the growing CNT.

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