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Optimal approach trajectories for a hydrogen donation tool in positionally controlled diamond mechanosynthesis

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Abstract

The use of precisely applied mechanical forces to induce site-specific chemical transformations is called positional mechanosynthesis, and diamond is an important early target for achieving mechanosynthesis experimentally. A key step in diamond mechanosynthesis (DMS) may employ a Ge-substituted adamantane-based hydrogen donation tool (HDon) for the site-specific mechanical hydrogenation of depassivated diamond surfaces. This paper presents the first theoretical study of DMS tool-workpiece operating envelopes and optimal tool approach trajectories for a positionally controlled hydrogen donation tool during scanning-probe based UHV diamond mechanosynthesis. Trajectories were analyzed using Density Functional Theory (DFT) in PC-GAMESS at the B3LYP/6- 311G(d, p)//B3LYP/3-21G(2d, p) level of theory. The results of this study help to define equipment and tooltip motion requirements that may be needed to execute the proposed reaction sequence experimentally and provide support for early developmental targets as part of a comprehensive near-term DMS implementation program.

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Keywords

Adamantane, Carbon, Diamond, DMS, Donation, Germanium, Hydrogen, Mechanosynthesis, Nanotechnology, Positional Control, Reaction Sequence, Trajectory