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Optimal tooltip trajectories in a hydrogen abstraction tool recharge reaction sequence for 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) employs an ethynyl-based hydrogen abstraction tool (HAbst) for the site-specific mechanical dehydrogenation of H-passivated diamond surfaces, creating an isolated radical site that can accept adatoms via radical-radical coupling in a subsequent positionally controlled reaction step. The abstraction tool, once used (HAbstH), must be recharged by removing the abstracted hydrogen atom from the tooltip, before the tool can be used again. This paper presents the first theoretical study of DMS tool-workpiece operating envelopes and optimal tooltip trajectories for any positionally controlled reaction sequence-and more specifically, one that may be used to recharge a spent hydrogen abstraction tool-during scanning-probe based ultrahigh-vacuum 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

Abstraction, Carbon, Diamond, DMS, Germanium, Hydrogen, Mechanosynthesis, Nanotechnology, Pathology, Positional control, Reaction sequence, Tooltip, Trajectory