Molecular Manufacturing Gallery

DC10c Carbon-transfer Tooltip

Description:
Damian Allis and Eric Drexler performed density functional theory quantum chemical analyses of the DC10c tooltip as a model system for carbon dimer transfer. This tooltip is featured in the nanofactory movie, “Productive Nanosystems: From molecules to superproducts”, which is available on YouTube and Google Video. Starting at the human scale, the viewer zooms in through a scale factor of a billion to follow molecules as they are sorted, bound, transformed, and joined to form larger and larger parts of a billion-processor laptop computer. The production and much of the animation design was done by John Burch of LizardFire Studios.

Authors:
Damian G. Allis
Department of Chemistry, Syracuse University
K. Eric Drexler
Nanorex, Inc. Hydrogen Abstraction Tooltip

Description:
The key difference between solution-phase chemistry and molecular manufacturing (MM) is the use of the directed positioning of tooltips and workspaces to fabricate or modify nanosystems in MM. Hydrogen abstraction tooltips are structures that can remove single hydrogen atoms from workspaces, thereby generating reactive sites onto which other atoms can be placed. The structure at left shows the product of a hydrogen abstraction process-a single hydrogen atom at the top of a diamondoid tetrahedron. Such processes are explored in section 8.5.4 of the book Nanosystems: Molecular Machinery, Manufacturing, and Computation .

Author:
K. Eric Drexler
Nanorex, Inc. Single-atom Deposition Tooltip

Description:
The ultimate control over the properties of any structure lies in the manipulation of individual atoms. Molecular manufacturing approaches that employ single-atom methods in nanosystem fabrication represent the highest level of design control and assembly flexibility achievable in nanotechnology. Molecular dynamics simulations of complete tooltip assemblies, such as shown at left, are performed to determine the positional accuracy possible with single-atom deposition methods.

Author:
Damian G. Allis
Department of Chemistry, Syracuse University DC10c Carbon-transfer Tooltip in detail Description:
The DC10c tooltip is a structure meant to stably bind carbon dimers (red) on a framework (grey) that can be embedded within diamondoid nanostructures through direct covalent carbon-carbon bonds. Upon carbon-dimer deposition, stability is imparted to the binding face of the tooltip by way of electronic conjugation between the dimer-binding carbon atoms (grey) and two conjugated pi-systems on either side (blue). The quantum chemical study of the DC10c tooltip, “Design and Analysis of a Molecular Tool for Carbon Transfer in Mechanosynthesis ” is available online from the Journal of Computational and Theoretical Nanoscience .

Authors:
Damian G. Allis
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Nanorex, Inc. A potential C100GeATD defect structure

Description:
A recent computational survey of candidate structures for carbon dimer deposition (Horizontal Ge-Substituted Polymantane-Based C2 Dimer Placement Tooltip Motifs for Diamond Mechanosynthesis , in press in the Journal of Computational and Theoretical Nanoscience) identified a number of germanium-based structures that may stably bind carbon dimers. These candidate structures provided the test systems for the NanoHive@Home Q-SMAKAS project, aimed at using molecular dynamics to generate possible tooltip defects. One such defect for the C100GeATD base structure (shown top) was found to occur by dimer bending and hydrogen abstraction from a nearby atom (bottom).

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