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Heterogeneous PEGylation of Diamond Nanoparticles

Supplementary Information—Visualization of Unique Attachment Sites

A. S. Barnard
Molecular & Materials Modelling, Data61, CSIRO, Docklands VIC 3008, Australia
amanda.barnard@data61.csiro.au

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This document contains visualisations of the unique attachment sites for polyethylene glycol (PEG) on a 1502 atom diamond nanoparticle, enclosed by a combination of {100}, {110} and {111} facets. The left column, throughout the document, depicts PEGylation configurations on a clean, reconstructed "bucky-diamond". The right column depicts the identical sites, visualise from the same orientation, for the corresponding hydrogen terminated nanodiamond. The pairs of configurations (clean and passivated) are not labelled, as labels are entirely arbitrary (configuration 1, configuration 2, configuration 3, ... etc). The goal here is to illustrate how PEG binds to the nanodiamond, and to provide a quick comparison between the two surface treatments, to highlight the impact of hydrogen passivation (or surface reconstructions) on the orientation of PEG. Missing images for hydrogen passivated configurations are due to the rebinding of those surface sites to the sub-lattice, and their subsequent inaccessibility to PEG, in each case.