Anisotropic Adsorption and Distribution of Immobilized Carboxyl on Nanodiamond

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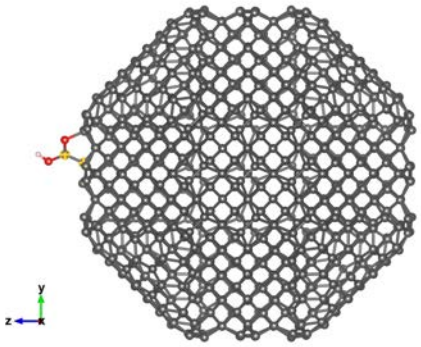
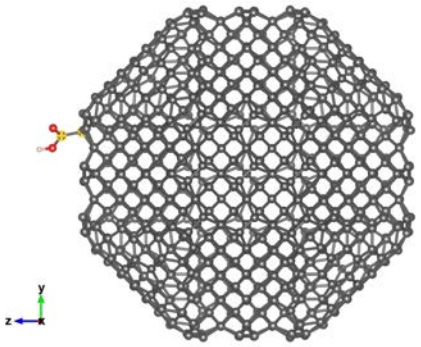
Electronic Supplementary Information

Configurations for COOH adsorbed on all sites within the irreducible surface area, of nanodiamonds with 1502 C atoms, which is equivalent to a hydrostatic diameter of 2.9 nm. This fully relaxed and reconstructed "clearn" bucky-diamond structure is provided to accompany this document. By exploiting the symmetry of the model structure the number of geometrically and crystallographically unique adsorption sites from 460 to 26. This underlying nanodiamond structure is enclosed entirely by $\{110\}$, $\{111\}$, and $\{100\}$ facets (in order of prevalence) and has an effective surface-to-volume ratio of $q = 1.031 \times q_0$, where q_0 is the surface to volume ratio of a sphere of equivalent mass.

All structures have been relaxed using the density functional tight-binding method with self-consistent charges (SCC-DFTB), which is an approximate quantum chemical approach where the Kohn–Sham density functional is expanded to second order around a reference electron density (obtained from self-consistent density functional calculations of weakly confined neutral atoms within the generalized gradient approximation (GGA)). The confinement potential is optimized to anticipate the charge density and effective potential in molecules and solids. A minimal valence basis set is used to account explicitly for the two-center tight-binding matrix elements within the DFT level, which is basis independent. The double counting terms in the Coulomb and exchange–correlation potential, as well as the intra-nuclear repulsion are replaced by a universal short-range repulsive potential. All structures have been fully relaxed with a conjugate gradient methodology until forces on each atom was minimized to be less than 10^{-4} a.u. (i.e. ≈5 meV/Å). In all the calculations, the "PBC" set of parameters is used to describe the contributions from diatomic interactions of carbon.



$d_{ND-COOH}$ = 1.4372Å



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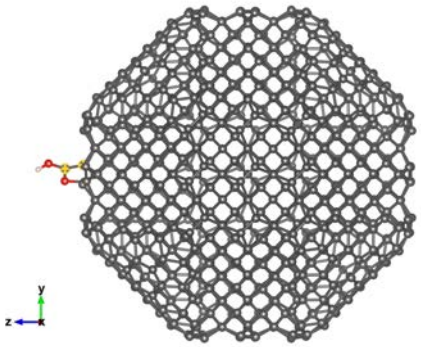

$d_{ND-COOH}$ = 1.4372Å

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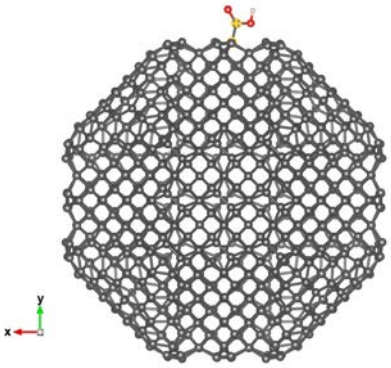

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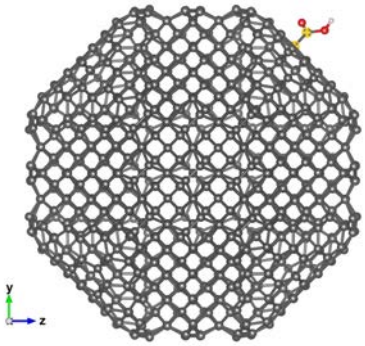

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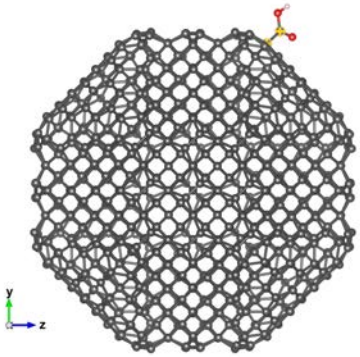

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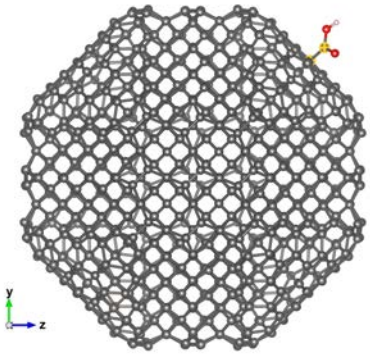

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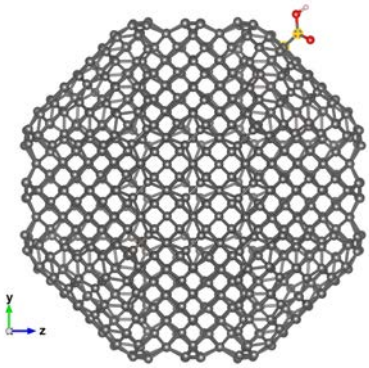

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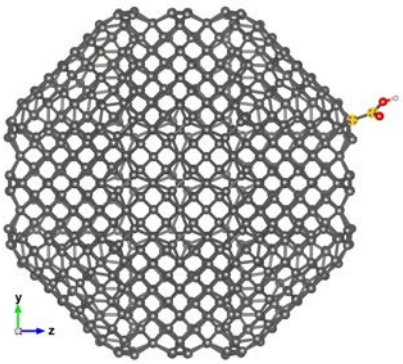

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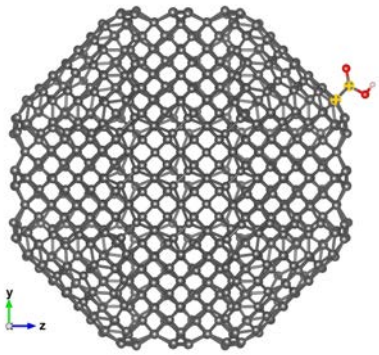

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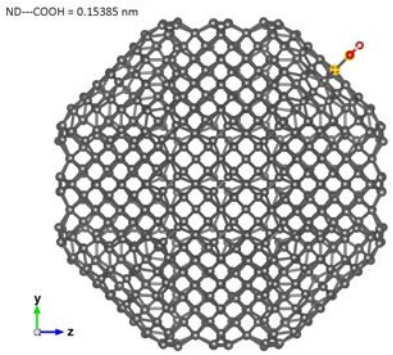

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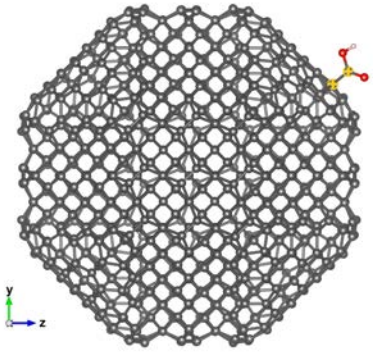

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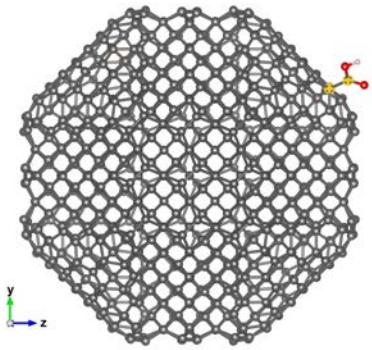

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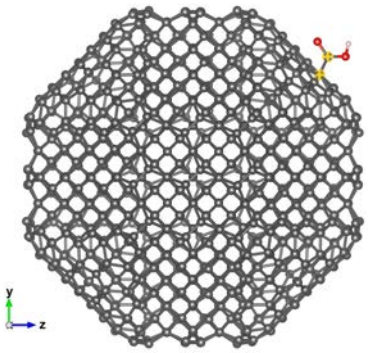

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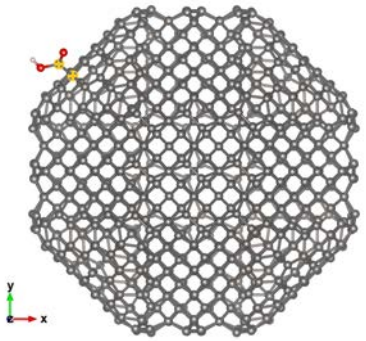

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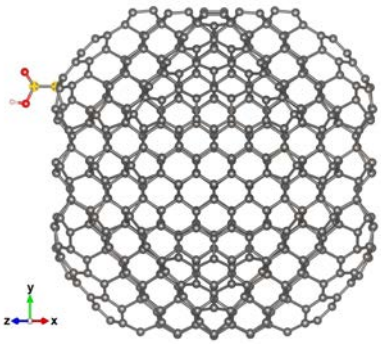

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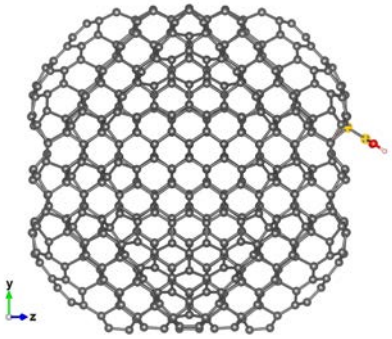

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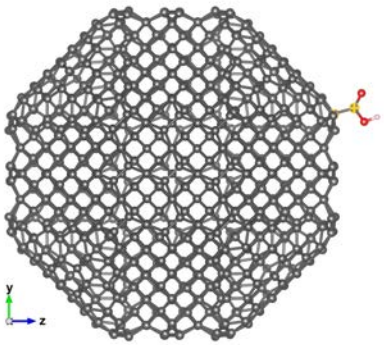

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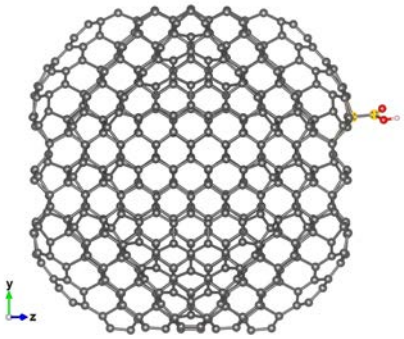

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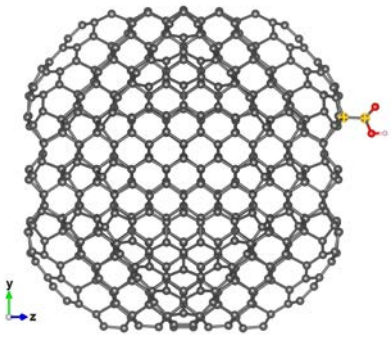

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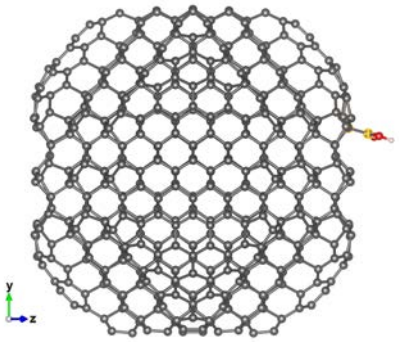

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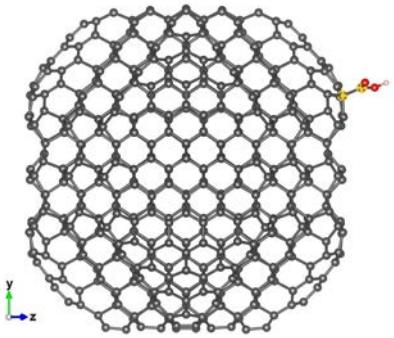

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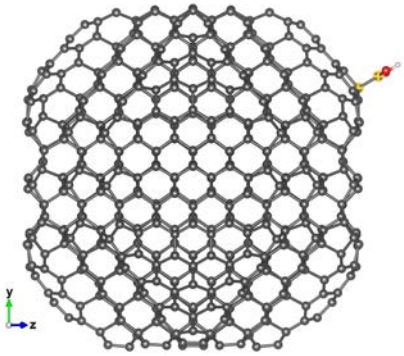

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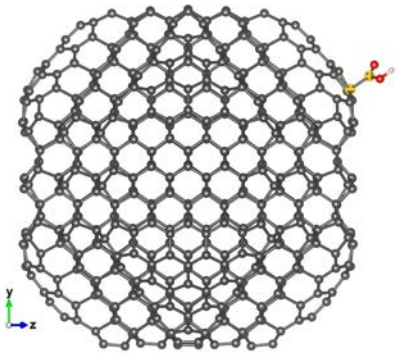

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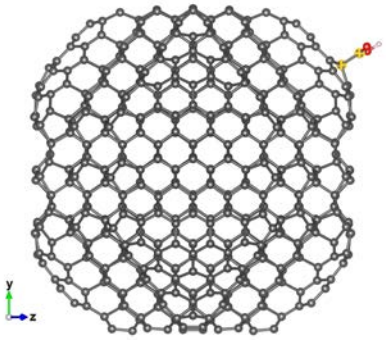

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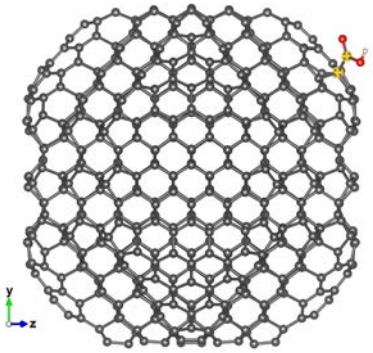

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