Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Atomically Precise Understanding of Nanofluids: Nanodiamonds and Carbon Nanotubes in Ionic Liquid

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Interaction models for nanoparticles

Trimantane diamondoid, $C_{18}H_{24}$, was modeled using the OPLS-based potential as devised elsewhere.[1] (5,5) CNT, 1.1nm long, was modeled using the OPLS force field as devised elsewhere.[2]

Table S1: Lennard-Jones-12-6 parameters and electrostatic partial charges Partial charges for the nanodiamond was obtained using ChelpG scheme, as described at reference 1. See Figure S1 for designation of the interaction sites.

Carbon nanotube	sigma, nm	epsilon, kJ mol^{-1}	charge, e
C	0.3314	0.414220	0.00
H*	0.2420	0.125520	0.00
Nanodiamond (Trimantane)			
C1	0.3550	0.317984	Ref. 1
C2	0.3550	0.317984	Ref. 1
C3	0.3800	0.209200	Ref. 1
H*	0.2420	0.125520	Ref. 1

* Saturation of the carbon atoms with hydrogen is natural corresponding to real, experimentally determined structures. Hence, usage of hydrogen atoms at the edges is chemically relevant. However, the interaction potentials on the hydrogen atoms in ND and CNT are different. The electrostatic potential on the surface of nanodiamonds is proven to be non-zero. Therefore, hydrogen atoms must carry a certain electrostatic charge. In turn, the simulated CNT models are much shorter than real CNTs. The ratio of the hydrogen atoms to the carbon atoms in real CNTs is negligibly small (unlike in trimantane nanodiamonds). Not to overestimate the role of the hydrogen atoms in CNT, they were simulated with zero electrostatic charges. Hereby the simulated CNT model was represented as a sidewall only, i.e. without the effects of caps and terminating atoms.

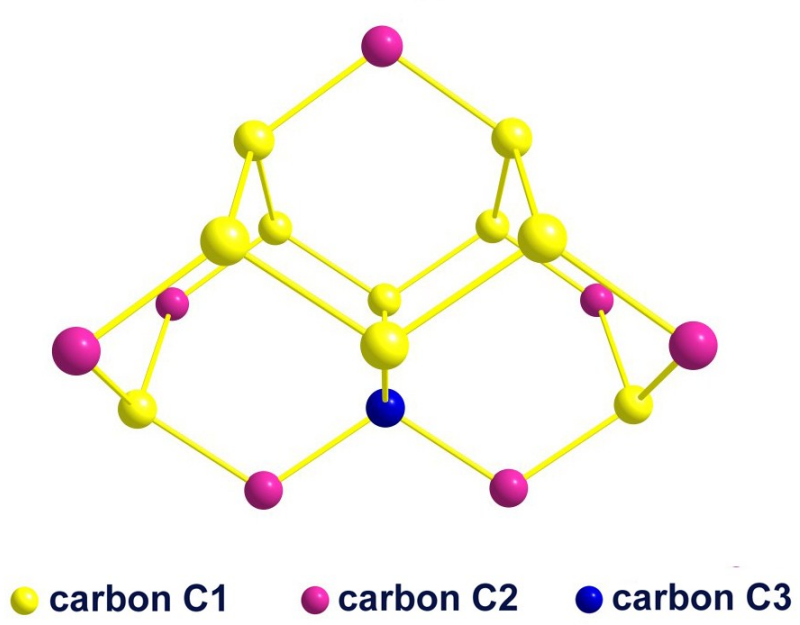

Figure S1: Designation of the interaction sites in nanodiamond (trimantane).

REFERENCES

1) Prediction of the Hydration Properties of Diamondoids from Free Energy and Potential of Mean Force Calculations, C. Maciel, T. Malaspina, and E. E. Fileti, J. Phys. Chem. B, 2012, 116 (45), pp 13467–13471. DOI: 10.1021/jp3079474

2) Polypeptide A9K at nanoscale carbon: a simulation study, Vitaly V. Chaban, Andre Arruda and Eudes Eterno Fileti, Phys. Chem. Chem. Phys., 2015, 17, 26386-26393. DOI: 10.1039/C5CP04565G