

Controlling the Electronic Properties of Nanodiamonds via Surface Chemical Functionalization: A DFT Study

Supporting Information

Noam Brown and Oded Hod

Department of Chemical Physics, School of chemistry, The Raymond and Beverly Sackler Faculty of Exact Sciences, Tel-Aviv University, Tel-Aviv 69978, Israel

Relative Stability

In Fig. 2 of the main text we presented the relative stability of the various systems considered as calculated at the HSE/6-31G** level of theory. Here, for completeness, we provide similar results obtained using the LDA and PBE exchange-correlation functional approximations. As can be seen in Fig. S1 below, similar trends are predicted by all functional approximations with somewhat higher relative stabilities obtained using the LDA.

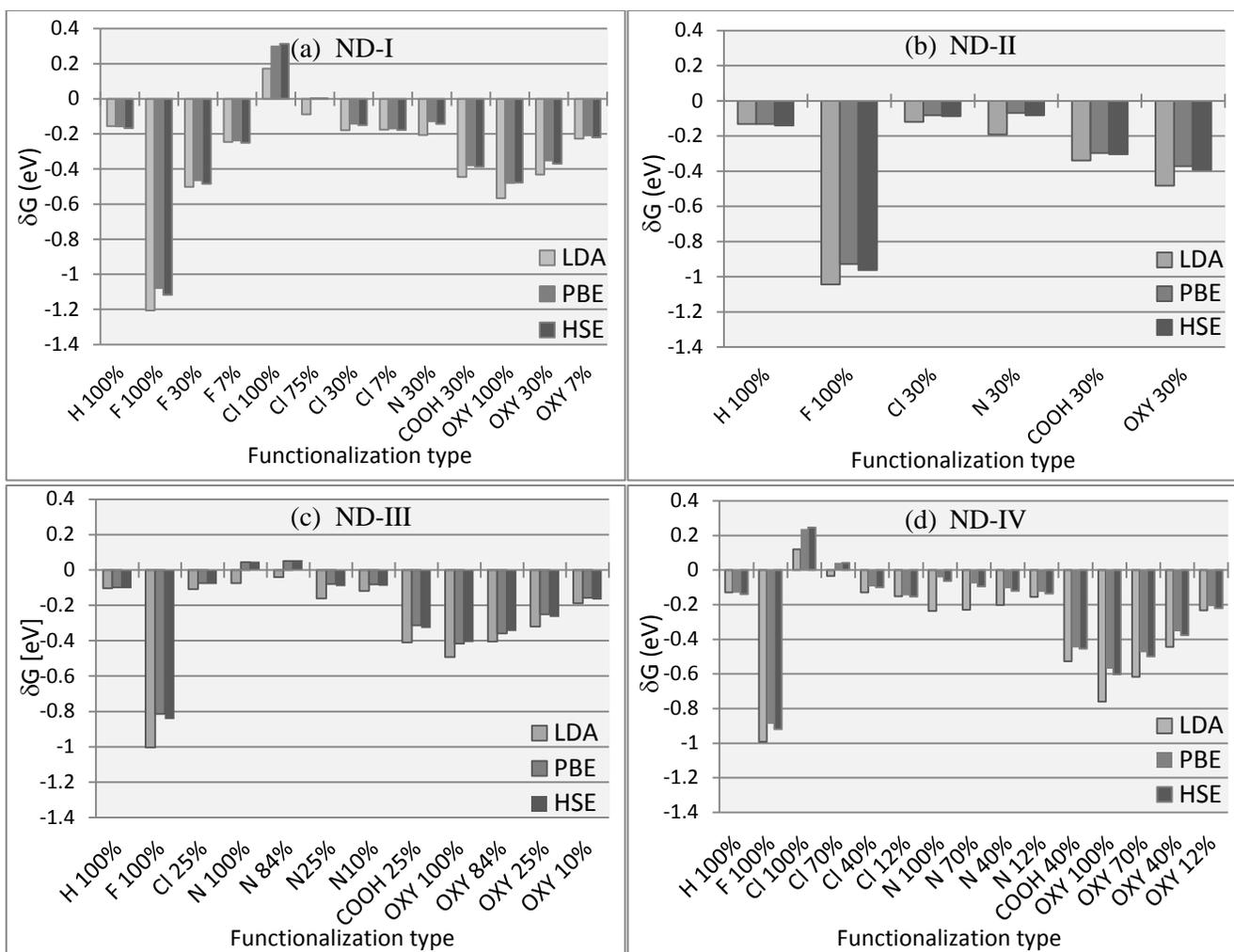


Figure S1: comparison of δG values, calculated using Eq. (1) of the main text, and obtained using the LDA, PBE, and HSE exchange correlation DFT functional approximations and the 6-31G** Gaussian basis-set for various surface functionalization schemes of the (a) ND-I, (b) ND-II, (c) ND-III, and (d) ND-IV systems.

Electronic Properties

In Fig. 3 of the main text we presented the HOMO-LUMO gaps of the various systems considered as calculated at the HSE/6-31G** level of theory. Here, for completeness, we provide similar results obtained using the LDA and PBE exchange-correlation functional approximations (see Fig. S2). As may be expected, the gaps obtained using the LDA and PBE functionals are similar (usually slightly smaller for LDA) and smaller than the values obtained using the screened-exchange hybrid HSE exchange-correlation functional approximation.

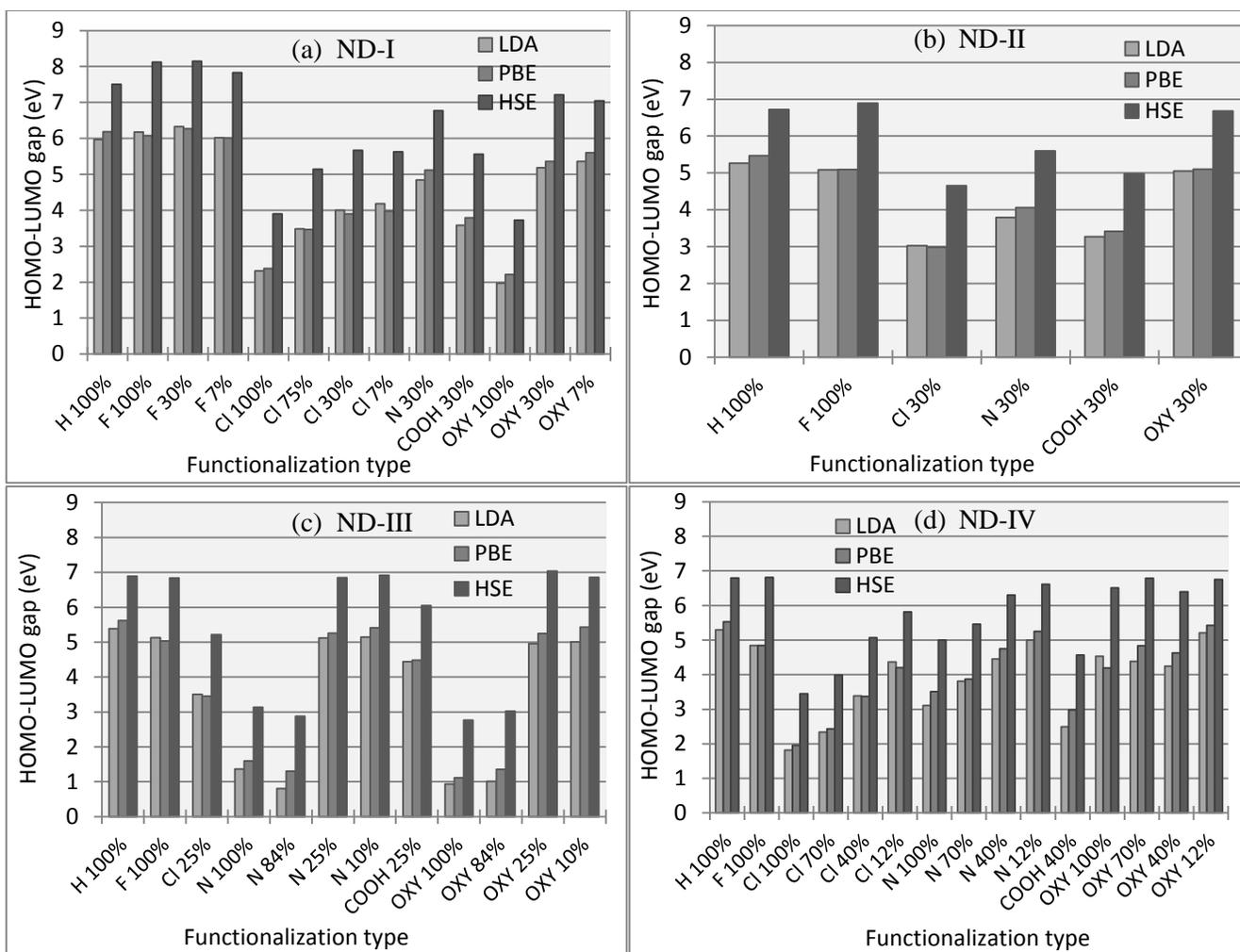


Figure S2: comparison of HOMO-LUMO gaps of the (a) ND-I, (b) ND-II, (c) ND-III, and (d) ND-IV systems as calculated using the LDA, PBE, and HSE exchange-correlation functional approximations and the 6-31G** Gaussian basis-set.