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Properties of Nitrogen-doped nanodiamond probed by first-principles. JEAN-YVES RATY, University of Liege, GIULIA GALLI, Lawrence Livermore National Laboratory — Nanodiamonds have been obtained as isolated clusters (in products of detonation and on some meteoritic samples) as well as aggregates in films produced by CVD. The incorporation of nanodiamonds into devices relies on the possibility of N-doping them efficiently. In this study, we report on the properties of Nitrogen-doped nanodiamonds (up to 1.5 nm in diameter) studied by ab initio molecular dynamics. Simple chemical potential calculations indicate that nitrogen incorporates into the surface. Extrapolation of our calculations for C29, C66 and C147-based clusters indicate that nitrogen atoms could incorporate substitutionally in the particle's core when the nanodiamonds diameter reaches ∼10nm. We discuss the energy of the donor levels of N-doped nanodiamonds together with their possible negative electron affinity, depending on surface reconstructions and nanoparticle size. Our ab-initio results point at the possibility of reaching effective electron emission from nanodiamonds. This work was performed under the auspices of the US Department of Energy by the University of California at the LLNL under contract no W-7405-Eng-48. JYR acknowledges support from the Belgian FNRS.

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