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Erratum: Density functional theory study on the B doping and B/P codoping of Si nanocrystals embedded in SiO_2 [Phys. Rev. B 95, 075307 (2017)]

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In the original paper, the beginning of the second paragraph of Sec. I reads “In contrast to the doping of hydrogen-passivated Si NCs, the doping of Si NCs embedded in SiO_2 has not been systematically simulated because complicated models need to be used in the simulation [32–35]. Guerra and Ossicini [36] and Carvalho *et al.* [37] investigated the doping of B and P in Si NCs that were passivated by OH groups.” Here, the statement on the models used by Guerra and Ossicini is not fully consistent with the description in Ref. [36]. In fact, Guerra and Ossicini used Si NCs embedded in SiO_2 for the study of B or P single doping and OH-passivated Si NCs for the study of B/P codoping. We would like to point out that no defects such as dangling bonds were at the Si/SiO_2 interface in their models of Si NCs embedded in SiO_2. But the original paper has highlighted that a dangling bond at the Si/SiO_2 interface plays an important role in the doping of Si NCs. In addition, the sizes of Si NCs embedded in SiO_2 were up to 1.2 nm (Si_{47}) in Ref. [36], while a size of 1.4 nm (Si_{71}) is used for our Si NCs embedded in SiO_2. The larger NC size in our paper is closer to those ($\gtrsim$2.0 nm) routinely obtained in experiments for Si NCs embedded in SiO_2. This facilitates a more reliable comparison between calculations and experiments. Please note that the present Erratum does not affect the results and conclusions of our original paper.

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