Abstract Submitted
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Near-infrared luminescent cubic silicon carbide nanocrystals for in vivo biomarker applications: an ab initio Study[1] ADAM GALI, VIKTOR ZÓLYOMI, Wigner Research Center for Physics, Hungarian Academy of Sciences, BÁLINT SOMOGYI, Budapest University of Technology and Economics — Small molecule-sized fluorescent emitters are needed as probes to image and track the locations of targeted nano-sized objects with minimal perturbation, and are much sought-after to probe biomolecules in living cells. For in vivo biological imaging, fluorescent biomarkers have to meet the following stringent requirements: (i) they should be non-toxic and bioinert, (ii) their hydrodynamical size should be sufficiently small for clearance, (iii) they should be photo-stable. Furthermore, it is highly desirable that (iv) they have intense, stable emission in the near-infrared range, and (v) they can be produced in relatively large amount for biological studies. Here we report time-density functional calculations on SiC-based QDs in the aspect of in vivo biological imaging applications. We find that Si-vacancy, divacancy, as well as single metal dopants such as Vanadium (V), Molybdenum (Mo) and Tungsten (W) in molecule-sized (1-2 nm) SiC QDs emit light efficiently in the near-infrared range. Furthermore, their emission wavelength varies on the size of host SiC QDs at less extent than that of pristine SiC QDs, thus sharper emission spectrum is expected even in a disperse size distribution of these QDs. These fluorescent SiC QDs are paramagnetic in the ground state.

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