First-principles calculation of the persistent spin helix on an OH-terminated diamond surface

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The surface termination of semiconductors is a key factor to overcome instability and chemical reactivity due to the dangling bonds. Hydrogen (H)-terminated diamond surfaces become more electrically conductive.[1,2] On the other hand, oxygen (O)-terminated diamond surfaces exhibit nonconductive electrical characteristics.[3] Additionally, the roughness of a diamond (111) surface with an O termination tends to be higher.[4] The OH termination may address concerns of such roughness.[5] We calculated the effect of the OH termination on the spin splitting on diamond surfaces by using first-principles calculations. Our calculation predicted that the OH-terminated diamond (111) surface exhibits the persistent spin helix (PSH) with a spin-orbit coupling coefficient α_{PSH} of 14.2 meV・Å. We also calculated the Rashba spin splitting on an H-terminated diamond surface with a Rashba coefficient α_R of 3.6 meV・Å. The α_{PSH} of an OH-terminated diamond surface is significantly larger than the α_R of an H-terminated one. OH-terminated diamond surfaces with in-plane electric polarization and mirror symmetry may generate a PSH state which is useful for spintronic devices.

References:

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