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Accurate electronic structures for Ce doped SiAlON using a semilocal exchange-correlation potential

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White light-emitting diodes (LEDs), the so-called next-generation solid-state lighting, offer benefits in terms of reliability, energy-saving, maintenance, safety, lead-free, and eco-friendly. Recently, rare-earth-doped oxynitride or nitride compounds have attracted a great deal of interest as a photo-luminescent material because of their unique luminescent property, especially for white LEDs applications. Ce doped β -SiAlON has been studied as a wavelength conversion phosphor in white LEDs thanks to its high absorption rates, high quantum efficiency, and excellent thermal stability. Previously researches were not enough to understand the detail mechanism and characteristics of β -SiALON. The bandgap structures and electronic structures were not exact due to limitation of calculation methods . In this study, to elucidate the Ce doping effect on the SiAlON system, accurate band structures and electronic structure of the Ce doped β -SiAlON was intensively investigated using density functional theory calculations. In order to get a better description of the band gaps, MBJLDA method were used. We have found a single Ce atom site in β -SiAlON super cell. Furthermore, the density of state, band structure and lattice constant were intensively investigated.

Keywords: SiAlON, MBJLDA, vasp, DFT