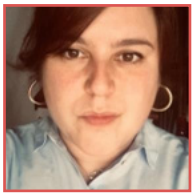
5th World Conference on
Advanced Materials, Nanoscience and Nanotechnology
May 20-21, 2024 | Rome, Italy
https://doi.org/10.62422/978-81-970328-7-5-020

Bulk and Monolayer WSe_2 and the Effect of the V Doping



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Tungsten diselenide (WSe_2) is a material that has captured the attention of researchers due to its unique properties, the proposed study focuses on the optical and electronic characteristics of WSe_2, by making use of the density functional theory (DFT) and employing Perdew-Burke-Ernzerhof (PBE) Generalized Gradient Approximation (GGA) density function and PseudoDojo pseudopotential. The study investigates the properties of both bulk and a monolayer of WSe_2 to determine how the number of layers affects the properties of the material. To further examine the peculiarities of WSe2, four different systems based on Vanadium doped-WSe2 have been investigated from the optical and electronic points of view. The systems contain different percentages of V: (i) WSe_2:V 1.4%, (ii) WSe_2:V 2.8%, (iii) WSe_2:V 5.6%, and (iv) WSe_2:V 11.2%. The introduction of Vanadium results in a reduction in the bandgap and a global shift of the projected density of the states. The Valence Band Maximum (VBM) also crosses the Fermi level, which is consistent with the p-type nature of vanadium doping. Furthermore, the absorption spectra change in terms of the position and the intensity of the optical transition as a result of the Vanadium introduction.

Biography:

Eleonora Pavoni got a PhD in chemistry, from the University of Bologna. During her PhD, she worked as a research fellow at the Institute of Organic Synthesis and Photoreactivity of the CNR, and then, she was a post-doc at the Biomedical and Neuromotor Sciences Department, University of Bologna. She has worked in the optical, Raman/IR spectroscopies field and material characterization by SPM Techniques. Currently, she is working at the Department of Matter, Environmental Sciences, and Urban Planning, of the Polytechnic University of Marche and her research is focused on the modeling and simulation of materials at the atomistic scale.