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NUMERICAL SIMULATION OF STRUCTURAL, ELECTRONIC AND OPTICAL PROPERTIES OF VANADIUM DISELENIDE (VSe₂)

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VSe₂ belongs to a group of compounds called transition metal dichalcogenides. This group of compounds have been exploited by several researchers both computationally and experimentally because of their intriguing properties such as low resistance, high chemical and mechanical stability, ease of synthesis among others that suites them for various applications ranging from catalysis, electronics, aerospace engineering to plasmonics just to mention a few which attracted our attention prompting us to investigate one of its members, that is VSe₂. In this regard, structural study of VSe₂ was undertaken using Perdew-Burke-Ernzerhof exchange correlation functional with two flavours of van der Walls correction namely Grimme (DFT-D2) and Tkatchenko-Scheffler (TS). This is because VSe₂ is layered material. From the structural data obtained PBE+DFT-D2 described the structural parameters of VSe₂ best. Vibrational properties via phonon calculations, mechanical properties via an elastic constant calculation and energetic properties via the calculation of formation and the cohesive energies confirm that VSe₂ is mechanically, dynamically and energetically stable in its trigonal phase. Furthermore, from carefully predicted electronic band structure and density of states, VSe₂ exhibits metallic character. Optical properties at the BSE level of approximation show that the compound is optically anisotropic with different absorption behaviour in-plane and out-of-plane. From the obtained values of the screened plasma frequency, VSe₂ is a promising plasmonic material.

Apply to be
 considered for a student
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Yes

Level for award
 (Hons, MSc,
   PhD, N/A)?

MSc

Main supervisor (name and email)
and his / her institution

Daniel Joubert, email address: Daniel.Joubert2@wits.ac.za , University of the Witwatersrand.

Would you like to
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Yes

Primary author: Mr RUGUT, Elkana (The National Institute for Theoretical Physics, School of Physics and

Mandelstam Institute for Theoretical Physics, University of the Witwatersrand, Johannesburg, Wits 2050, South Africa)

Co-author: Prof. JOUBERT, Daniel (The National Institute for Theoretical Physics, School of Physics and Mandelstam Institute for Theoretical Physics, University of the Witwatersrand, Johannesburg, Wits 2050, South Africa)

Presenter: Mr RUGUT, Elkana (The National Institute for Theoretical Physics, School of Physics and Mandelstam Institute for Theoretical Physics, University of the Witwatersrand, Johannesburg, Wits 2050, South Africa)

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