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Electronic, Optical, and Thermodynamic Properties of a Quantum Spin Liquid Candidate $NaRuO_2$: Ab-initio Investigation

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Abstract : Quantum spin liquids (QSLs), known for their competing interactions that prevent conventional ordering, exhibit emergent phenomena and exotic properties resulting from quantum correlations. Despite these recent advancements in QSLs, a significant portion of the optical and thermodynamic properties in the Kagome lattice remains unknown. In addition, the thermodynamic phenomenology of $NaRuO_2$ bears a resemblance to that of highly frustrated magnets. Here, we employed ab-initio calculations to explore the electronic, optical and thermodynamic properties of $NaRuO_2$, a new QSL candidate. $NaRuO_2$ was identified as a semiconductor with a small bandgap energy of 0.69 eV. Our results reveal huge anisotropic optical properties, in which a distinct refractive index within the ab-plane indicating an impressive birefringent character of the $NaRuO_2$ system and a significant enhancement of the optical absorption coefficient and optical conductivity in the in-plane with respect to the c-axis. The investigation also examines the electronic anisotropy of the gap energy; by applying strain, the gap energy displays significant variations in the ab-plane compared to the out-of-plane direction. Conversely, calculations of the thermodynamic properties reveal a low thermal conductivity (2.5-0.5 $W.m^{-1}.K^{-1}$) and specific heat, which suggests the existence of strong interactions among the $NaRuO_2$ quantum spins. The linear specific heat behavior observed in $NaRuO_2$ suggests the fractionalization of electrons and the presence of a spinons Fermi surface. These findings hold promising potential for future quantum applications.

Keywords : quantum spin liquids, anisotropy, hybrid-DFT, applied strain, optoelectronic and thermodynamic properties
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