Spin current generation in 2D metallic transition metal dichalcogenides and their Janus systems in presence of light

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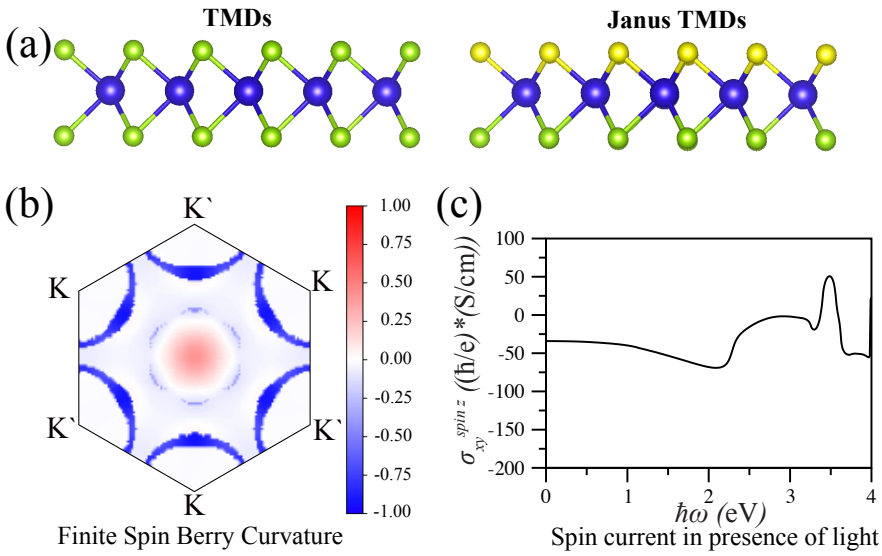
A pure spin current generation is one of the central phenomena in the field of spintronics due to its potential for low energy consumption in next-generation electronics [1]. Non-magnetic materials with prominent spin-orbit-coupling (SOC) strength can produce spin-current [2]. Metallic transition metal dichalcogenide (TMD) monolayers from group-VI (such as $NbSe_2$, $TaSe_2$, TaS_2 and NbS_2) have been both theoretically and experimentally shown to possess an Ising-type SOC field [3]. Owing to this Ising-type SOC, these systems can exhibit finite spin-Berry curvature (SBC). Here, using first-principles calculations, we explore the properties of this finite SBC to generate pure spin current in the presence of light. We find that monolayers with Se atoms, such as $TaSe_2$ and $NbSe_2$, exhibit high spin current conductivity around 2-3 eV of incident photon energy owing to their anisotropic spin-splitting [4]. Furthermore, we explore effect of Rashba SOC by making Janus TMDs i.e., NbSSe and TaSSe in spin current generation. Therefore, these systems can have significant potential applications in spintronic devices.



Finite Spin Berry Curvature

Spin current in presence of light

References:

[1] *Nat. Mater.* **11**, 382-390 (2012). [2]. *Nat. Comm.* **15**, 4362 (2024) [3]. *Phys. Rev. Lett.* **129**, 087002 (2022). [4] *J. Phys. Chem. C* **128**, 14514-14521 (2024).

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