Enhanced optical absorption in heterostructures formed by CdO and SnC monolayers

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Abstract

Assembling 2D materials in vertical heterostructures is one of the main techniques for enhancing electronic and optical properties. In most cases, known as van der Waals heterostructures (vdWHs), the interlayer distances are larger than typical covalent bond lengths resulting in weak interlayer interactions. It has been shown that reducing the distance between the layers can significantly alter the properties of separated layers, which is not so noticeable in vdWHs and thus creates a new platform for controlling the physical properties of 2D materials [1]. Such structures are rarely reported in the literature. Examples are borophene/ graphene [2] and ZnO/ MgO [3] heterostructures.

Motivated by the enhanced properties of 2D vertical heterostructures, we employed ab-initio calculations based on density functional theory and examined CdO/SnC systems in four different stackings. Our results reveal that despite of thermodynamic and mechanical stabilities of all considered structures, according to calculated phonon frequencies, only the structure formed by placing the Sn atom on top of the O atom and the C atom on top of the Cd atom is dynamically stable at zero Kelvin. This structure has an interlayer distance of 2.52 Å which is smaller than the interlayer distance in typical vdWHs. We also investigated the electronic and optical properties of this dynamically stable structure utilizing the GW+BSE approach. Unlike the monolayer CdO which possesses a single optical absorption peak close to the red light energy, the considered CdO/SnC structure has an optical bandgap of 1.14 eV, and it can absorb 13% of incident light in the blue light region.

References

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[2] Seyedmohammadzadeh, Mahsa, Cem Sevik, and O□uz Gülseren, Physical Review Materials, 6 (2022) 104004.
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Figures

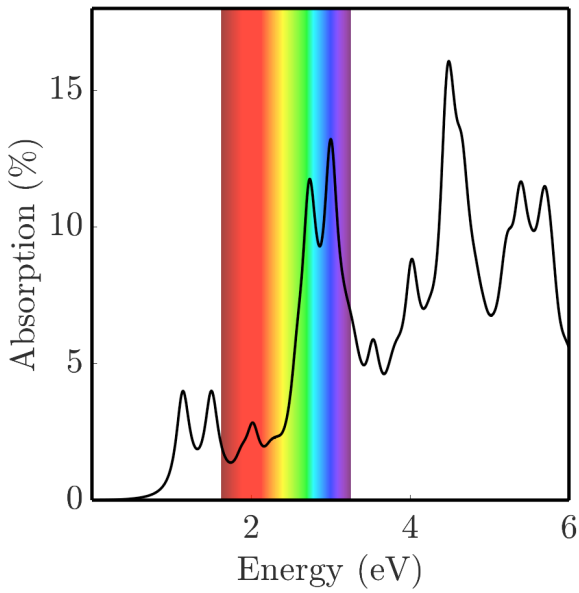

Figure 1: Optical absorption of the dynamically stable CdO/SnC heterostructure for perpendicular incident light.