**First-Principles Investigation of the Optical Properties of Layered Phyllosilicates**

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In recent years, the focus of the 2D materials community has increasingly shifted toward phyllosilicates—a diverse group of naturally occurring van der Waals layered minerals. These materials display a broad spectrum of electronic, magnetic, and optical properties, many of which remain under active investigation. Their intrinsic robustness and stability under ambient conditions further enhance their appeal for various applications.

Talc, the most well-known member of the phyllosilicate family, is a wide-band-gap insulator characterized by a highly anisotropic crystal structure. It comprises stacked TOT layers—two tetrahedral (T) sheets strongly bonded to a central trioctahedral (O) sheet—held together by weak van der Waals forces [1]. The octahedral sheet consists of magnesium-centered octahedra, while the tetrahedral sheets contain silicon–oxygen units, arranged to reinforce the layered integrity of the structure. Remarkably, talc retains its structural and electronic stability even when exfoliated down to the monolayer limit.

This work investigates the optical properties of phyllosilicates, with a particular focus on talc. First-principles calculations were carried out using the Quantum ESPRESSO package [2], based on density functional theory (DFT) with plane-wave basis sets and projector augmented-wave (PAW) pseudopotentials. Exchange-correlation interactions were treated using the PBE-GGA functional, and Grimme-D2 van der Waals corrections were included to account for interlayer interactions. Optical response was evaluated at the random phase approximation (RPA) level. Current efforts aim to expand this study to other phyllosilicate species, supporting their potential use in optoelectronics, nanocomposites, and 2D heterostructure engineering.

REFERENCES

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