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First-principles study of optical aspects of penta-graphene monolayer under strain effects

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In this study, based on the first-principles calculations using the Density Functional Theory (DFT) employing Wien2k computing codes, the optical properties of penta-graphene such as the joint density of states, the real and imaginary part of the complex dielectric function, absorption, and reflectivity spectrum under special conditions such as strain effects, are studied. The behavior of the optical aspects of penta-graphene is analyzed. It can be concluded that this monolayer is suitable for use in designing optoelectronic devices, especially as sensors under the proposed conditions.

Keywords: First-principles calculations, Density Functional Theory (DFT), Optical properties, Strain effects