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Interlayer Interaction Arising from Lone Pairs in s-Orbitals in 2D Materials

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Abstract : Interlayer interactions or hybridization in van der Waals (vdW) heterostructures of two-dimensional (2D) materials significantly influence their physical characteristics, including layer-dependent electronic and vibrational structures, magic-angle superconductivity, interlayer antiferromagnetism, and interlayer excitons. These interactions are sensitive to a set of interdependent and externally tunable parameters. To fully exploit the potential of these materials, it is crucial to understand the physical origins of interlayer interaction and hybridization. Traditional theories often attribute these interactions to the sharing of electrons via p orbital lone pairs or π electrons, based on the octet rule, which posits that p electrons are the primary occupants of the outermost atomic shells, except in hydrogen. However, our study challenges this prevailing belief. Through high-throughput screening and density function theory, we demonstrate that s orbital lone pairs can also drive interlayer interactions in 2D materials. The crystal field and inert pair effect induce a Stark-like phenomenon, leading to energy level splitting and the formation of directional electron clouds. This allows these electrons to directly participate in the hybridization of interlayer wavefunctions without forming chemical bonds. Our findings expand the understanding of interlayer interactions, revealing new mechanisms that govern these properties and providing a theoretical foundation for manipulating interlayer phenomena in 2D materials.

Keywords : interlayer interaction, nanomaterials, 2D materials, van der waals, heterostructures
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