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"Phantom" Modes in *Ab Initio* Tunneling Calculations: Implications for Theoretical Materials Optimization, Tunneling, and Transport
SERGEY V. BARABASH, DIPANKAR PRAMANIK, Intermolecular Inc. — Development of low-leakage dielectrics for semiconductor industry, together with many other areas of academic and industrial research, increasingly rely upon *ab initio* tunneling and transport calculations. Complex band structure (CBS) is a powerful formalism to establish the nature of tunneling modes, providing both a deeper understanding and a guided optimization of materials, with practical applications ranging from screening candidate dielectrics for lowest "ultimate leakage" to identifying charge-neutrality levels and Fermi level pinning. We demonstrate that CBS is prone to a particular type of spurious "phantom" solution, previously deemed true but irrelevant because of a very fast decay. We demonstrate that (i) in complex materials, phantom modes may exhibit very slow decay (appearing as leading tunneling terms implying qualitative and huge quantitative errors), (ii) the phantom modes are spurious, (iii) unlike the pseudopotential "ghost" states, phantoms are an apparently unavoidable artifact of large numerical basis sets, (iv) a presumed increase in computational accuracy increases the number of phantoms, effectively corrupting the CBS results despite the higher accuracy achieved in resolving the true CBS modes and the real band structure, and (v) the phantom modes cannot be easily separated from the true CBS modes. We discuss implications for direct transport calculations. The strategy for dealing with the phantom states is discussed in the context of optimizing high-quality high-κ dielectric materials for decreased tunneling leakage.

Sergey V. Barabash
Intermolecular Inc.

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