

Effect of ZBL potential on kinks in repulsive lattices.

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Supersonic kinks have been shown to exist in lattices where the interaction between particles or atoms is only repulsive and the atoms are kept inside the system because of external forces. Theory and numerical experiments show that the velocities and energies of kinks diverge when the amplitude of the kinks approaches the interatomic distance.

It is however unrealistic the fact that for large energies the atoms become too close. At those distances the overlapping of the electron wavefunction produces strong repulsion that is modeled with empirical short range potentials. Considering the applicability of the repulsive lattice to the interlayer potassium sheet in silicates, we calculate and use the Ziegler-Biersack-Littmark (ZBL) potential between the potassium ions and study the consequences on kink properties, both numerically and analytically. The main conclusion is that kinks propagate with large energy having however realistic distances between them.