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Method Comparison for Calculating Properties of Charged Ferroelectric Domain Walls

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We consider two approaches when calculating the properties of a ferroelectric system with charged domain walls. These properties include domain wall width, electronic band structure and occupancy, and the electronic potential energy. Previously, a single parameter, Q , was argued to determine the crossover of the electron gas from quantum to quasi-classical. However, to obtain this result, two simplifying approximations were made in the description of the domain wall. When compared with a more robust approach it appears these approximations are only valid for a low Q value system. We discuss why these approximations are not always valid depending on the material parameters, i.e. the Landau theory parameters.

Keyword-1

Ferroelectric

Keyword-2

Quantum

Keyword-3

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