How good is DFT in determining structural properties of 2D ferroelectrics?

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Over the past few years, my group has been investigating peculiar two-dimensional transformations taking place in ultrathin ferroelectrics [1-3]. While discrepancies on electronic structure can be relatively small across many exchange-correlation functionals, *structural energy differences*—in between ground states and a structure with higher symmetry—*can vary by orders of magnitude*, so that it may be fair to say that no precise knowledge of these energy differences, or of the appropriate functional, is available yet. *Ab initio* approaches in which exchange and correlation are included exactly appear to be necessary.

Determining energy differences with increased precision is necessary in theories that explain experimentally-observed phenomena in which two-dimensional ferroelectrics become paraelectrics [4] in a quantitative (parameter-free) manner. Additionally, knowing the value of these energy differences becomes crucial to determine if potential two-dimensional quantum paraelectric or paraelastic phases may exist [5,6].

References:

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