Ewald summation on a helix: A route to self-consistent charge density-functional based tight-binding modeling of helical structures

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We present the generalization to helical case of the classical Ewald method [1], the harbinger of all modern self-consistent treatments of waves in crystals, including ab initio electronic structure methods. The derived formulas for the electrostatic potential and van der Waals energy prove to be numerically tractable and thus capable to provide the crucial component needed for coupling objective molecular dynamics [2] with the machinery of self-consistent charge density-functional based tight-binding [3]. The resultant method is put to work in illustrative simulations on a helical boron nitride nanotube, a screw dislocated zinc oxide nanowire, and an ideal DNA strand.

We will discuss in more depth the case of twisted zinc oxide nanowires and nanotubes, which were recently synthesized by screw-dislocation growth. We show [4] that the existence of these structures can be rationalized in terms of the energetics of surfaces and veritable Eshelby's twist linear elasticity mechanics supplemented by a nonlinear core term.

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