

Total-energy pseudopotential calculations: using ABINIT

Vipin Mishra, Chinmaya Pandey



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Total-energy pseudopotential calculations: using ABINIT Vipin Mishra, Chinmaya Pandey There is a little doubt that most of low-energy physics, chemistry and biology can be explained by thequantum mechanics of electrons and ions. The limits of applicability and even the interpretation of thepredictions of modern quantum theory are lively areas of debate among philosophers. Questions such as "How do we interpret the probabilistic nature of wave functions?", "What constitutes a measurement?,""How much can we ever know about the state of a system?," and "Can quantum mechanics describeconsciousness?" are of fundamental importance. Despite the fact that these questions are still debated, it isclear that whether or not a more complete description of the world is possible, those things that modernquantum theory does predict are predicted with incredible accuracy.

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