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Electronic Structure of Matter: Wave Functions and Density Functionals

Walter Kohn*

Keywords: COST · Density functional theory · Wave functions

Traditionally, since about 1930, the electronic structure of matter has been described by Schroedinger wave functions (WF). More recently an alternative formulation known as density functional theory (DFT) has been developed, which describes electronic structure in terms of the electronic density distribution, n(r). DFT was recognized by a Nobel Prize in 1998.

In this talk I have tried to convey the strengths and weaknesses of DFT in comparison with WF methods. DFT provides a new conceptual perspective on electronic structure. Its practical usefulness lies in its ability to deal with systems of O(1000) atoms compared with O(10-100) atoms for WF methods. For small systems, WF methods are more reliable and accurate.

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