Density-Functional Theory and its Applications

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November this year marks fifty years since the publication of the Hohenberg–Kohn theorems, which laid down the formal foundations of density-functional theory (DFT). Since that time, DFT has become an invaluable tool for many researchers across a range of disciplines. It is therefore highly timely to present this themed collection, published in conjunction with the *15th International Conference on Density-Functional Theory and its Applications (DFT2013)*. This conference took place at Durham University, UK, from 9–13 September 2013 and was attended by 216 delegates from 35 countries. It was the latest in a series of biennial meetings that have taken place most recently in Madrid (2001), Brussels (2003), Geneva (2005), Amsterdam (2007), Lyon (2009), and Athens (2011).

The collection presents a snapshot of contemporary DFT research, highlighting the interplay between theory development, applications and experiment, and illustrating the diversity and impact of the method. The papers range across fundamental theory and applications, on topics including energy functionals, time-dependent DFT (TDDFT), spin properties, electric and magnetic properties, intermolecular interactions, conceptual DFT, catalysis and chemical reactivity, molecular dynamics and computer algorithms. The systems investigated include idealised models, molecules, surfaces and periodic solids. The collection also contains Perspectives on dye chemistry with TDDFT, one-electron self-interaction and the asymptotics of the Kohn–Sham potential, and density functional tight binding, written by leading researchers in these fields. We are very grateful to all the authors who have contributed to this collection.

The next edition of this biennial conference series will take place in Debrecen, Hungary, in 2015, some fifty years after the publication of Kohn–Sham theory, which converted the formal foundations of Hohenberg and Kohn into a practical computational scheme.

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