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BOOK REVIEW

Kaplan, I. G.: Intermolecular Interactions: Physical Picture, Computational Methods, and Model Potentials

Wiley, 2006, 367 + xii pages. $180.00 in hardcover

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This book has a remarkably broad coverage of molecular interactions, primarily noncovalent ones; it is up to date, and it presents many topics with a better perspective than one usually encounters. The book contains qualitative descriptions of all kinds of physical interactions: electrostatic, inductive, and dispersion-like; long-, intermediate-, and short-range; and chemical, physical, and biological. This is supplemented by enough mathematics to satisfy most physical chemists. The book covers computational approaches as well as theoretical foundations, and an attempt is made to cover even the most recent state-of-the-art literature. There are also brief discussions on covalent bonding, repulsion, and interactions of large bodies. An appendix presents an introduction to quantum chemical methods (including coupled cluster theory and density functional theory) for nonspecialists. There is also a practical introduction to methods for finding global minima of potential energy surfaces.

Here are some more specific comments. There is an excellent discussion on basis set superposition error, the best I have read so far. It is also admirable that the author makes a serious assessment of density functional theory for noncovalent interactions, including medium-range dispersion-like interactions. The discussion of many-body effects is important since intermolecular interactions in complex systems are not pairwise additive.

I very much liked the author's grounding the subject of the long-range multipole series properly in the context of asymptotic expansions. This allowed him to make the points that (1) there is an optimum term at which to truncate the series, and (2) the best way to add the terms is to stop with one-half of the smallest term. In my experience, these points are widely unappreciated. The author is very authoritative, and getting these details right is an example of his carefulness.

This is the best book I have ever seen on noncovalent interactions. I recommend this monograph to all those interested in intermolecular interactions.

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