DESCRIPTION

This book covers the theory and applications of continuum solvation models. The main focus is on the quantum-mechanical version of these models, but classical approaches and combined or hybrid techniques are also discussed.

• Devoted to solvation models in which reviews of the theory, the computational implementation

• Solvation continuum models are treated using the different points of view from experts belonging to different research fields

• Can be read at two levels: one, more introductive, and the other, more detailed (and more technical), on specific physical and numerical aspects involved in each issue and/or application

• Possible limitations or incompleteness of models is pointed out with, if possible, indications of future developments

• Four-colour representation of the computational modeling throughout.

ABOUT THE AUTHOR

Benedetta Mennucci and Roberto Cammi are the authors of Continuum Solvation Models in Chemical Physics: From Theory to Applications, published by Wiley.