Título: Continuum Solvation Models In Chemical Physics From Theory To Applications
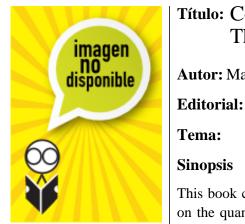
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Sinopsis

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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.