P04

Continuum Solvation for Finite and Infinite Periodic Systems in Crystal

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ABSTRACT

In this contribution, we present recent progress made in the generalized finite- difference continuum solvation model recently implemented in the CRYSTAL code [1,2], with applications both to finite molecular systems and infinite periodic ones such as polymers, nanotubes, helices, and surfaces.

In particular, the self-consistent reaction-field procedure used to compute the electrostatic contribution to the solvation energy has recently been extended to consider a variety of atomic charges models belonging to the Class II and Class IV families [3,4].

In addition, the Cavitation, Dispersion and Structural effects model [5] for non-electrostatic contributions to the solvation energy and related nuclear gradients has also been implemented [6] and reparametrized [7], together with a fully analytical procedure for the calculation of the solvent-accessible surface area and its nuclear gradients [8] which has been generalized to periodic systems [9].

We discuss application of the proposed continuum solvation model to selected finite and infinite periodic systems, compare its performances to reference continuum solvation models and present the main current areas of development and application currently considered.

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