

arXiv.org > physics > arXiv:1107.1655

Physics > Chemical Physics

Continual Model of Medium III: Calculation of analytical gradients of parameters of surface meshes on the molecular surfaces over atomic coordinates

Oleg Kupervasser, N. E. Wanner

(Submitted on 8 Jul 2011 (v1), last revised 16 Oct 2012 (this version, v3))

The problem of finding of analytical gradients (derivatives over atoms coordinates) of solvation energies can be decomposed on two subtasks: at the first stage we search for parameters of the superficial devices (three coordinates, three components of normal vector and square) and their derivatives; at the second stage we differentiate energy and we express it through derivative of the matrixes featuring a problem. But these derivatives of matrix elements can be expressed through derivatives of parameters of surface meshes of SES (solvent excluded surface) or SAS (solvent accessible surface). The purpose of the given paper is finding of these analytical gradients of the parameters of the surface meshes.

Comments:35 pages, 10 figures paper in English and in RussianSubjects:Chemical Physics (physics.chem-ph)Cite as:arXiv:1107.1655 [physics.chem-ph](or arXiv:1107.1655v3 [physics.chem-ph] for this version)

Submission history

From: Oleg Kupervasser [view email] [v1] Fri, 8 Jul 2011 15:10:21 GMT (657kb) [v2] Wed, 10 Aug 2011 11:44:37 GMT (656kb) [v3] Tue, 16 Oct 2012 21:19:22 GMT (831kb)

Which authors of this paper are endorsers?

Search or Article-id

All papers 🚽 Go!

(Help | Advanced search)

Download:

• PDF only

Current browse context: physics.chem-ph < prev | next > new | recent | 1107

Change to browse by:

physics

References & Citations

NASA ADS

