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Continual Model of Medium I: Algorithm for Formation of Smooth Molecular Surface

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In this paper the full and exhaustive algorithm of formation of a smooth molecular Solvent Excluded Surface- SES, and also Solvent Accessible Surface- SAS is presented. These surfaces are a boundary between molecule and solvent. The basis of the algorithm is primary and secondary rolling of molecules. Originality of the paper consists in making of the full and improved algorithm of secondary rolling which allows to create optimal smooth surface SES of any molecule or any set of molecules by rolling any irregularities and close to irregularities situations appearing during primary rolling. The adaptive critical distance characterizing maximal admissible irregularity of a surface is used. The main task, which will be solved by the formed surface and which will be considered in the further papers, is a calculation of solvation energy and its gradients for continual models of solvent. Also it can be used for the demonstration purposes in the molecular editors.

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