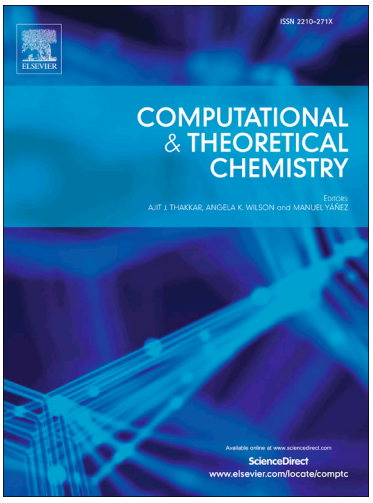

The interaction of proteins with silica surfaces. part I: Ab initio modeling

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The Interaction of Proteins with Silica Surfaces.

Part I: Ab Initio Modeling

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ABSTRACT

Recently synthesized 2D zeolites with well-defined external surfaces have been used as model systems for the adsorption of proteins on silica materials. In this work the interaction of 19 proteinogenic amino-acid side chains in the C representation and the Ace-NMe backbone model with the 2D-UTL and 2D-MWW zeolites has been investigated. The performance of different DC-DFT methods has been compared against the MP2/CBS and CCSD(T)/CBS levels of theory for cluster models of -quartz and 2D-UTL. The obtained statistics clearly indicate that none of the common DC-DFT methods is capable of describing the side-chain interaction with silica surfaces within chemical accuracy (~1 kcal/mol). Two different approaches have been employed to improve the accuracy: (i) the re-parameterization of the pair-wise dispersion term as proposed by Grimme 2006 and (ii) the correction scheme based on an error analysis of the vdW-DF2 functional. Both methods provide consistent and highly accurate results for external silica surfaces with and without silanol groups.