Using *ab initio* potential to predict thermodynamic properties of fluids and minerals

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Macroscopic thermodynamic properties (PVT properties, phase behavior, chemical potential, speciation reactions, enthalpy etc.) of fluids are determined by intermolecular, and to a less extent, intramolecular interactions, which are functions of molecular distances and angles. Here we present our two studies to demonstrate how to predict the thermodynamic properties through molecular level study.

(1) Using ab initio calculated molecular potentials of thousands of different configurations, predicting multi-phase equilibria of methane hydrate, liquid and vapor phases under conditions of different temperature, pressure, salinilty and pore sizes. Comparison with the experimental data shows that this model can accurately predict the equilibrium *p-T* condition of CH_4 hydrate in seawater and porous media with high accuracy.

(2) Based on molecular interaction potential for pure H_2O and CO_2 and the ab initio potential surface across CO_2–H_2O molecules, we carried out more than one thousand molecular dynamics simulations of the PVTx properties of the mixtures in the TP range from 673.15 to 2573.15 K up to 10.0 GPa. Comparison with extensive experimental PVTx data indicates that the simulated results generally agree with experimental data within 2% in density, equivalent to experimental uncertainty.

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Rock-Eval pyrolysis of the Água de Madeiros Formation (Lower Jurassic) from the Lusitanian Basin, Portugal

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The Lower Jurassic hemipelagic series in the Lusitanian Basin constitutes one of the most important intervals regarding the occurrence of potential hydrocarbon source-rocks in Portugal [1]. One of these units is the Água de Madeiros Formation (Upper Sinemurian to lowermost Pliensbachian), which is composed by organic-rich marl–limestone alternations with several black-shale horizons [2].

Based on the study of this unit in its type locality (S. Pedro de Moel area), about 58 m thick, we present in this work a high-resolution organic geochemical analysis centered in Rock-Eval pyrolysis. Total organic carbon (TOC), determined in more than 170 samples and covering the whole succession, shows a large variation and reaches up to 22 wt.%. A great part of the 78 analyzed samples by pyrolysis present S2 values above 10 mg HC/g rock, reaching a maximum of 78.1 mg HC/g rock. Moreover, these high S2 values are correlative with the highest recorded values of the Hydrogen Index, that shows an average around 400 mg HC/g TOC (maximum of 637 mg HC/g TOC).

Despite these interesting geochemical indicators in terms of good source-rock potential, thermal maturity of the Água de Madeiros Formation in the studied reference section is low (clearly immature), as suggested by T_{max} values always below 437 ºC.

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