Asphaltene interaction with calcite surface: A first principles study

RAPHAEL S. ALVIM[1], THOMAS F. HEADEN[2], EDO S. BOEK[2] AND CAETANO R. MIRANDA[13]

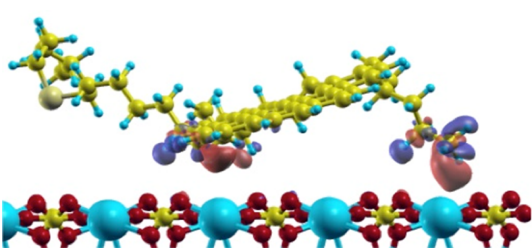
[1]Universidade Federal do ABC , Santo André, Brazil raphael.alvim@ufabc.edu.br

[2]Imperial College London, Dept. of Chemical Engineering, t.headen@imperial.ac.uk, e.boek@imperial.ac.uk

[3]Universidade de São Paulo, DFMT-IF, São Paulo, Brazil cmiranda@if.usp.br

Asphaltenes play a key role in the oil production and exploration. However, even their structure, precitation and deposition processes are not fully understood. These molecules can be the primary adsorbing species in oil mixtures, reducing the oil recovery process. The attractive forces that cause asphaltenes to associate and agglomerate can be induced due to asphaltene–rock surface interactions. In carbonate reservoirs, calcite (10-14) surface is regarded for retaining asphaltenes. Here, we use first principles calculations to study the asphaltene-surface interactions with calcite (10-14). The calculations are based on density functional theory (DFT) within GGA functional with van der Waals (vdW) dispersion correction. Asphaltene and resin models were obtained from previous studies [1]. These large molecules impose a very challenge description at this level. Our results suggests that although there is steric hindering in interaction of the aromatic ring region on the surface, the organic chains in asphaltene molecule plays a significant role on the adsorption process, mainly through vdW interactions. The adsorption energies were found to be favorable (~2.40 eV). With adsorption, a significant charge rearrangement was observable in the non-aromatic sites compared with the isolated molecules. The calcite (10-14) surface selectively adsorbs the most polar asphaltenes from oil and our studies provide a much needed description of these interactions at molecular level.

Charge density difference for asphaltene adsorbed on calcite surface relative to the isolated systems. Red (positive) and Blue (negative).



[1] T. F. Headen, *et al*., *Energy & Fuels* 2009, **23**, 1220.