XIX SBQT
Simpósio Brasileiro de Química Teórica 2017
12 a 17/Nov, 2017, Águas de Lindóia/SP, Brasil

# Adsorption of Benzoic Acid on Carbonate Surfaces

Authors: Filipe C. D. A. Lima[1,2], Raphael S. Alvim[1], Caetano R. Miranda[1]

*1. Departamento de Física dos Materiais e Mecânica, Instituto de Física, Universidade de São Paulo, São Paulo SP, Brasil. 2. Instituto Federal de Educação, Ciência e Tecnologia de São Paulo (IFSP), campus Matão, SP, Brasil*

**Abstract:** The adsorption of crude oil components through carboxylic acid groups may affect the water wettability of the carbonate reservoirs, usually composed by calcite $CaCO_3$ or dolomite $CaMg(CO_3)_2$ [1,2]. The Benzoic Acids (BA) binding nature and selectivity effects toward either calcite or dolomite are still unclear. We investigate the BA adsorption process on the $CaCO_3$ and $CaMg(CO_3)_2$ surfaces in the more stable plane (10-14), in the framework of the density-functional theory (DFT) [3], using the GGA exchange-correlation functional revised PBE (revPBE) with van der Waals (vdW) correction [4,5]. The adsorption of the BA molecule on *calcium* and *magnesium* sites were systematically analyzed for different conformations, as well dissociation products. The results show that BA can have distinct stable conformations on the carbonate surfaces through the carboxyl group with less influence of the aromatic ring. The molecule tends to be perpendicular with respect to the calcite surface, displaying strong interactions, mainly between the carboxyl group and both calcium and carbonate sites. However, for dolomite, although the perpendicular position is also the more favorable, the most selective interaction is between BA's carbonyl and surface magnesium sites. And it allows the BA's hydroxyl group to be free to interact. Our results also indicate that the BA-dolomite adsorption is influenced by interaction with water molecules. It is shown that the formation of the benzoate on the dolomite is more favored even in the absence of water molecules, increasing the selectivity of BA toward this surface. The obtained adsorption and dissociation landscape provide fundamental insights on the nature of the interaction of oil components and water wettability on carbonates systems with potential impact on oil recovery processes.

**Key-words**: DFT, Benzoic Acid, Benzoate, Calcite, Dolomite.
**Support:** This work has been supported by Petrobras, CNPq and Fapesp.

**References:**

[1] D. Konopacka-Łyskawa, B. Kościelska, and J. Karczewski, J. Cryst. Growth **418**, 25 (2015).

[2] K. Jarrahian, O. Seiedi, M. Sheykhan, M.V. Sefti, and S. Ayatollahi, Colloids Surfaces A Physicochem. Eng. Asp. **410**, 1 (2012).

[3] W. Kohn and L.J.J. Sham, Phys. Rev. **140**, A1133 (1965).

[4] M. Dion, H. Rydberg, E. Schröder, D.C. Langreth, and B.I. Lundqvist, Phys. Rev. Lett. **92**, 246401 (2004).

[5] G. Román-Pérez and J.M. Soler, Phys. Rev. Lett. **103**, 96102 (2009).