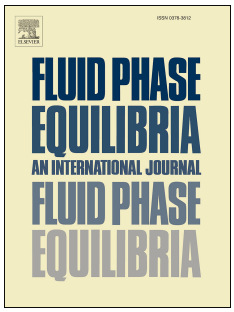


# Molecular dynamics simulation and experimental validation by X-ray data of hydroxyapatite crystalline structures

Carla L.M. Camargo, Neuman S. Resende, Carlos A.C. Perez, Charlles R.A. Abreu, Vera M.M. Salim, Frederico W. Tavares

PII: S0378-3812(17)30430-2

DOI: 10.1016/j.fluid.2017.11.007

Reference: FLUID 11642

To appear in: *Fluid Phase Equilibria*

Received Date: 2 September 2017

Revised Date: 31 October 2017

Accepted Date: 3 November 2017

Please cite this article as: C.L.M. Camargo, N.S. Resende, C.A.C. Perez, C.R.A. Abreu, V.M.M. Salim, F.W. Tavares, Molecular dynamics simulation and experimental validation by X-ray data of hydroxyapatite crystalline structures, *Fluid Phase Equilibria* (2017), doi: 10.1016/j.fluid.2017.11.007.

# Molecular dynamics simulation and experimental validation by X-ray data of hydroxyapatite crystalline structures

Carla L. M. Camargo[a], Neuman S. Resende[a], Carlos A. C. Perez[a], Charlles R. A. Abreu[b], Vera M. M. Salim[a], Frederico W. Tavares[a,b*]

[a] Programa de Engenharia Química, PEQ/COPPE, Universidade Federal do Rio de Janeiro, Centro de Tecnologia, Cidade Universitária, Rio de Janeiro, 21941-914, RJ, Brazil.

[b] Escola de Química, Universidade Federal do Rio de Janeiro, Centro de Tecnologia, Cidade Universitária, Rio de Janeiro, 21941-909, RJ, Brazil.

[*]Corresponding author. Tel.: +55 21 2562 7650; fax: +55 21 2562 7567.

E-mail adresses: cmanske@peq.coppe.ufrj.br (C.L.M. Camargo), tavares@eq.ufrj.br (F.W. Tavares)

**ABSTRACT.** Computer simulations have provide information about structural and dynamic properties of hydroxyapatite (HAp). However, the accuracy of simulated HAp in the description of experimental crystalline structures is not evaluated in many of theoretical studies. Here, molecular dynamics (MD) simulations of HAp in the isobaric-isothermal (NPT) ensemble are carried out using LAMMPS at temperature of 298K and pressure of 1atm. We evaluate the quality of two sets of force field parameters by comparison between simulated and experimental unit-cell geometry and powder X-ray diffraction (XRD) patterns. Presence of calcium vacancies is taken into account in the simulations in order to reproduce a non-stoichiometric HAp synthesized in our lab. By using the number of vacancies determined from X-ray fluorescence (XRF) results, we observe great similarity between experimental and simulated diffraction patterns and unit-cell parameters as well as in the atom positions inside the unit cell. Significant structural modifications are identified when an excessive number of calcium atoms was removed, which emphasizes the importance of considering reliable experimental data. We encourage the use of this experimental validation methodology to demonstrate the quality of any simulated crystalline structure.

**KEYWORDS.** Hydroxyapatite, MD simulations, experimental validation, XRD patterns

## 1. INTRODUCTION

Hydroxyapatite (HAp) [$Ca_{10}(PO_4)_6(OH)_2$] is a crystalline material of great interest in biology and the chemical industry. This material has been extensively investigated for biomedical applications due to its biocompatibility [1,2]. High stability and flexibility of HAp structure enable cationic/anionic substitutions and enhance its application as catalyst and adsorbent of heavy metals [3–7].