Combined Molecular Dynamics Simulations and Experimental Studies of the Removal of Cationic Dyes on Eco-friendly Adsorbent of Activated Carbon Decorated Montmorillonite Mt@AC .

Hassan Ouachtak *[a,b], Anouar El Guerdaoui [c], Rachid El Haouti [c], Redouane Haounati [a], Hamza Ighnih [a], Yahya Toubi [a,b], Fadi Alakhras [d], Rabia Rehman [e], Naima Hafid [f], Abdelaziz Ait Addi **[a], Mohamed Labd Taha [a].

[a] Laboratory of Organic and Physical Chemistry, Faculty of Science, Ibn Zohr University, Agadir, Morocco
[b] Faculty of Applied Science, Ait Melloul, Ibn Zohr University, Agadir, Morocco
[c] Department of Chemistry, Faculty of Science, Ibn Zohr University, Agadir, Morocco
[d] College of Pharmacy, Middle East University, Amman, 11831, Jordan
[e] Institute of Chemistry, University of the Punjab, Lahore-54590, Pakistan
[f] Regional Center of Education and Training Souss Massa, Morocco

Author for correspondence to: ouachtakhassan@gmail.com

aitaddi.abdelaziz@gmail.com

Phone number: +212669731920

S1. Characterization

All samples were characterized by Fourier transform infrared spectroscopy in the range of 4000–400 cm^{-1} using an ABB Bomem FTLA 2000 spectrometer with 16 cm^{-1} resolution. XRD measurements were recorded on a Bruker AXS D-8 diffractometer using Cu-Ka radiation in Bragg–Brentano geometry (q–2q). SEM micrographs were obtained on a Tecnai G2 microscope at 120 kV. The surface areas of the prepared materials were measured using the Brunauer–Emmett–Teller (BET) method on a 3Flex automatic analyzer. Prior to N_2 sorption, all samples were degassed at 250 °C for 8 h. The elemental composition of the sample was confirmed by energy dispersive spectroscopy EDS. Mappings showing elemental composition and surface distribution were obtained using the SEM-EDS method. The zeta potential of the Mt@AC composite was measured by microelectrophoresis techniques using a Zeta-Sizer Nano series (Malvern Instrument).

S2. Description of COMPASS Force Field

The COMPASS (**C**ondensed-phase **O**ptimized **M**olecular **P**otentials for **A**tomistic **S**imulation **S**tudies) is a member of the consistent family of force fields (CFF91, PCFF, CFF and COMPASS), which are closely related second-generation force fields. They were parameterized against a wide range of experimental observables for organic compounds Containing H, C, N, O, S, P, halogen atoms and ions, alkali metal cations, and several biochemically important divalent metal cations. PCFF is based on CFF91, extended so as to have a broad coverage of organic polymers, (inorganic) metals, and zeolites. COMPASS is the first force field that has been parameterized and validated using condensed phase properties in addition to various and empirical data for molecules in isolation. Consequently, this forcefield enables accurate and simultaneous prediction of structural, conformational, vibrational, and thermo-physical properties for a broad range of molecules in isolation and in condensed phases. The COMPASS force field consists of terms for bonds (b), angles (θ), dihedrals (ϕ), out-of-plane angles (χ) as well as cross-terms, and two non-bonded functions, a Coulombic function for electrostatic interactions and a Lennard-Jones potential for van der Waals interactions. [1]–[3]

$$E_{\text{total}} = E_b + E_\theta + E_\phi + E_\chi + E_{b,b'} + E_{b,\theta} + E_{b,\phi} + E_{\theta,\phi} + E_{\theta,\theta'} + E_{\theta,\theta',\phi} + E_q + E_{\text{vdW}}$$

where

$$E_b = \sum_b \left[k_2(b-b_0)^2 + k_3(b-b_0)^3 + k_4(b-b_0)^4\right]$$
$$E_\theta = \sum_\theta \left[k_2(\theta-\theta_0)^2 + k_3(\theta-\theta_0)^3 + k_4(\theta-\theta_0)^4\right]$$
$$E_\phi = \sum_\phi \left[k_1(1-\cos\phi) + k_2(1-\cos 2\phi) + k_3(1-\cos 3\phi)\right]$$
$$E_\chi = \sum_\chi k_2\chi^2$$
$$E_{b,b'} = \sum_{b,b'} k(b-b_0)(b'-b'_0)$$
$$E_{b,\theta} = \sum_{b,\theta} k(b-b_0)(\theta-\theta_0)$$
$$E_{b,\phi} = \sum_{b,\phi} (b-b_0)\left[k_1 cos\phi + k_2 cos2\phi + k_3 cos3\phi\right]$$

[1] M. J. McQuaid, H. Sun, and D. Rigby, "Development and validation of COMPASS force field parameters for molecules with aliphatic azide chains," *J. Comput. Chem.*, vol. 25, no. 1, pp. 61–71, Jan. 2004, doi: 10.1002/jcc.10316.

[2] H. Sun, "COMPASS: An ab Initio Force-Field Optimized for Condensed-Phase ApplicationsOverview with Details on Alkane and Benzene Compounds," *J. Phys. Chem. B*, vol. 102, no. 38, pp. 7338–7364, Sep. 1998, doi: 10.1021/jp980939v.

[3] J. Yang, Y. Ren, A. Tian, and H. Sun, "COMPASS Force Field for 14 Inorganic Molecules, He, Ne, Ar, Kr, Xe, H_2, O_2, N_2, NO, CO, CO_2, NO_2, CS_2, and SO_2, in Liquid Phases," *J. Phys. Chem. B*, vol. 104, no. 20, pp. 4951–4957, May 2000, doi: 10.1021/jp992913p.