Sociedad Cubana de Física y Facultad de Física, Universidad de La Habana

FÍSICA
REVISTA CUBANA DE FÍSICA

Supplementary Information:

Clayff Force Field Versus TIP3P Water Model in Molecular Simulations: Validation for Montmorillonite Clay Model

Información suplementaria:

Campo de Fuerzas Clayff Versus Modelo de Agua TIP3P en Simulaciones Moleculares: Validación para el Modelo de Arcilla Montmorrillonita

A. Lam[a)] & G. Rojas-Lorenzo[b)]

[a)] Zeolite Engineering Laboratory, Institute of Material Science and Technology (IMRE), University of Havana, Havana, CP. 10400, Cuba

[b)] Instituto Superior de Tecnologías y Ciencias Aplicadas, Universidad de La Habana, Ave. Salvador Allende y Luaces, Quinta de Los Molinos, Plaza, La Habana 10600, Cuba

PACS: Molecular dynamics calculations (cálculos de dinámica molecular), 31.15.xv; Solvent effects (efectos solventes), 31.70.Dk; Potential energy surfaces (superficies de energía potencial), 31.50.Bc.

Citation: A. Lam, and G. Rojas-Lorenzo, Rev. Cubana Fis. **39**, 85 (2022)

https://www.revistacubanadefisica.org/index.php/rcf/article/view/2022v39p085

Supporting information

Lennard-Jones (L-J) potential was used to represent the van der Waals term in the total energy of the system.

$$E_{LJ} = \sum_{i \neq j} 4\,\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right]$$

This potential combines the short-range repulsion associated with atom-atom overlap and the short-range attraction associated with electron dispersion and it is calculated in CLAYFF and AMBER force fields by the following expresion:

$$E_{VDW} = \sum_{i \neq j} \varepsilon_{ij}^{*}\left[\left(\frac{\sigma_{ij}^{*}}{r_{ij}}\right)^{12} - 2\left(\frac{\sigma_{ij}^{*}}{r_{ij}}\right)^{6}\right]$$

while it is a little modified in CHARMM force fields as

$$E_{VDW} = \sum_{i \neq j} \varepsilon_{ij}^{*}\left[\left(\frac{\sigma_{ij}^{*}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}^{*}}{r_{ij}}\right)^{6}\right]$$

The ε_{ij}^{*} and σ_{ij}^{*} can be determined using standard arithmetic or geometry (Lorentz-Berthelot) combining rules. In CLAYFF, CHARMM and AMBER force fields,is d ε_{ij}^{*} etermined using standard geometric combination rule and u σ_{ij}^{*} sing standard arithmetic combination rule:

$\varepsilon_{ij}^{*} = \left(\varepsilon_{i}^{*}\,\varepsilon_{j}^{*}\right)^{1/2}$ and $\sigma_{ij}^{*} = \frac{\sigma_{i}^{*} + \sigma_{j}^{*}}{2}$ for all these used force fields.

Table SI1. Charges and atomic parameters for van der Waals interactions.
$\varepsilon_{ij}^{*} = \varepsilon_{ij}$ and $\sigma_{ij}^{*} = 2^{1/6}\,\sigma_{ij}$.

	symbol	charge (*e*)	ε_{0i} (kcal/mol)	σ_i (Å)
Clay	Si[a]	2.1000	1.8405×10^{-6}	3.3020
	Mg[a]	1.36	9.0298×10^{-7}	5.2643
	Li[a]	0.525	9.0298×10^{-7}	4.2101
	Li+[b]	1.0000	0.6700	2.3370
	F[b]	-0.8109	0.1802	3.1170
	O[a]	-1.0500	0.1554	3.1655
	Oo[a]	-1.1808		
	Oh[c]	-0.95		
	H[c]	0.425		
water SPC	HW[d]	0.4100		
	OW[d]	-0.8200	0.1553	3.5533
water TIP3P	HW[e]	0.417		

	OW[e]	-0.834	0.1521	3.53650
Oh-H Morse Potential[c]	$U(r) = E_0[\{1 - \exp(-k\,(r_{ij} - r_0\,))\}^2 - 1]$			
	E_0 (kcal/mol)	k ($Å^{-1}$)	r_0 (Å)	
	132.2491	2.1350	0.9450	

[a] R. T. Cygan, J.-J. Liang, and A. G. Kalinichev, J. Phys. Chem. B **108**, 1255 (2004).
[b] S. Koneshan, J. C. Rasaiah, R. M. Lynden-Bell, and S. H. Lee, J. Phys. Chem. B **102**, 4193 (1998).
[c] M. Pouvreau, J. A. Greathouse, R. T. Cygan, and A. G. Kalinichev, J. Phys. Chem. C **123**, 11628 (2019).
[d] H. Berendsen, J. P. M. Postma, W. van Gunsteren, and J. Hermans, *Interaction models for water in relation to protein hydration.* In *Intermolecular Forces*, (Pullman, B., Ed.; D. Reidel: Amsterdam, 1981) pp. 331.
[e] W. L. Jorgensen, J. Chandrasekhar, J. D. Madura, R. W. Impey, and M. L. Klein, J. Chem. Phys. **79**, 926 (1983).

Table SI2. Volume, Temperature and Total Configurational Energy (Eng-conf) average values (Av) and the standard deviation (σ) for the simulations.

Systems	Temperature (K)		Volume ($Å^3$)		Eng-conf (kcal/mol)	
	Av	σ	Av	σ	Av	σ
CLAYFF-water SPC	300.28	2.75	123687.60	200.92	-779591.20	71.40
CLAYFF-water TIP3P	300,05	2,77	123145,33	184,56	-779669.72	69.31