

# Force Field Parameterization via Atoms-in-Molecules

Alexander Pérez de la Luz<sup>1</sup>, Jorge Alberto Aguilar-Pineda<sup>1</sup>, José Guillermo Méndez-Bermúdez<sup>2</sup>, and José Alejandre<sup>1</sup>

<sup>1</sup> Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa. Av. San Rafael Atlixco 186, Col. Vicentina, Ciudad de México 09340, México

<sup>2</sup> Centro Universitario de los Valles, Universidad de Guadalajara, Carretera Guadalajara-Ameca km. 45.4, Ameca, Jalisco 46600, México

Having good force fields of polar liquids is fundamental to understand, from molecular point of view, several phenomena in a wide range of scientific and technological applications in chemistry, physics, biology and engineering. In recent works it has been shown that force fields such as OPLS/AA [1], GAFF [2] and CGenFF [3] fail to reproduce the miscibility of liquids with different degree of polarization [4]. We will present in this work a new route to assign the charge distribution of atoms in molecules based in the total molecular density (Hirshfeld) [5]. This methodology is applied a 10 polar liquids in pure component, the liquids have a dielectric constant going from 15 to 180 are studied using a systematic procedure to obtain the interaction parameters of a new all atoms force field [6]. The simulation results for dielectric constant, surface tension, liquid density, heat of vaporization and self-diffusion coefficient at room conditions have excellent agreement with experimental data, and they are also tested in binary mixtures, which shows the power of the method.

**Table 1. Average Relative Error,  $|X_{\text{exp}} - X_{\text{MD}}|*100/X_{\text{exp}}$ , between Calculated and Experimental Values for the 10 Polar Liquids Studied in This Work<sup>a</sup>**

Property	NEWFF	OPLS/AA	GAFF	CGenFF	OPLS16
Dielectric Constant	3.4	52.6	37.6	42.8	28.8
Surface Tension	2.7	10.5	26.1	22.1	20.7
Density	0.29	1.8	4.1	3.2	2.6
Heat of Vaporization	4.5	3.4	16.3	9.9	5.7
Self-Diffusion	19.2	37.4	49.0	60.6	32.9
Shear Viscosity	21.8	16.6	52.2	35.2	14.0
Isothermal Compressibility	11.6	8.7	27.5	19.2	25.5
Volumetric Expansion Coefficient	15.5	6.2	8.0	4.0	13.4

## Bibliography.

- 1 Jorgensen, W. L.; Tirado-Rives, J. *J. Am. Chem. Soc.* **110**, 1657-1666, 1988.
- 2- Wang, J. ; Wolf, R. W.; Caldwell, J. W.; Kollman, P. A. *J Comp. Chem.* **25**, 1157-1174, 2004.
- 3.- Vanommeslaeghe, K.; Hatcher, E.; Acharya, C.; Kundu, S.; Zhong, S.; Shim, J.; Darian, E.; Guvench, O.; Lopes, P.; Vorobyov, I.; Mackerell A. D. Jr. *J Comput. Chem.* **31**, 671-690, 2010.
- 4.- de la Luz, A. P.; Méndez-Maldonado, G. A; Núñez-Rojas; Alejandre, J. *J. Chem. Theory Comput.* 2015, **11** (6), 2792–2800
5. – Hirshfeld, F. L *Theoret. Chim. Acta.* **44**, 129-138, 1977
- 6.- Salas, F. J.; Méndez-Maldonado, G. A; Núñez-Rojas, E.; Alejandre, José *J. Chem. Theory Comput.* **11** , 683–693, 2015