Projecte de Treball Fi de Màster (TFM)

Màster en Modelització Computacional Atomística i Multiescala en Física, Química i Bioquímica
UB/UPC

Títol	**Anàlisi del punt crític de la transició de fase líquid-líquid en el model 3D de molts cossos per a l'aigua**
Title	**Critical point analysis for the liquid-liquid phase transition for the 3D many-body water model**

Director	**Giancarlo Franzese**
Departament	**Física Fonamental**
Universitat	**UB**
Tutor[1]	

Curs	**2015-16**

Summary[2]

Water is characterized by the hydrogen-bond interaction that has an important many-body component, usuallynot included in atomistic non-polarizable models. Here we consider a model that is coarse-grained in such a way to include this many-body component. We study the phase diagram for the 3D model with specific attention to elucidate the occurrence of the hypothesized liquid-liquid phase transition and to characterize the corresponding liquid-liquid critical point.

Keywords[3]: water; liquid-liquid phase transition; liquid-liquid critical point; many-body interactions; hydrogen bonds.

Breu descripció del projecte[4]

Water has many anomalies, all possibly related to the peculiar network of hydrogen bonds that the water molecules form. This interaction has an important many-body component, due to cooperativity [1], that is not included in pair-wise additive atomistic potentials, but that has been investigated recently for the case of a water monolayer [2]. It has been shown, by studying the response functions and the correlation length, that at low temperature the monolayer undergoes a liquid-liquid (LL) phase transition ending in a critical point in the universality class of the two-dimensional (2D) Ising model. The existence of a LL critical point has been suggested as a possible explanation for the water's anomalies [3]. Here we will investigate, by efficient Cluster Monte Carlo simulations (**STEP 1**) combined with the Histogram Reweighting Method and Finite Size Scaling Analysis (**STEP 2**), if the model has the LL critical point in 3D and to which universality class it belongs. The implications of this work could be relevant for our understanding of water's phase diagram that, despite its importance for our life, is still the object of a strong debate [4, 5, 6].

[1] Stokely, K., Mazza, M. G., Stanley, H. E. & Franzese, G. Effect of hydrogen bond cooperativity on the behavior of water. Proc. Natl. Acad. Sci. USA 107, 1301(2010).
[2] Bianco, V. & Franzese, G. Critical behavior of a water monolayer under hydrophobic confinement. Sci. Rep. 4, 4440 (2014).
[3] Poole, P. H., Sciortino, F., Essmann, U. & Stanley, H. E. Phase-Behavior Of Metastable Water. Nature 360, 324 (1992).
[4] Limmer, D. T. & Chandler, D. The putative liquid–liquid transition is a liquid–solid transition in atomistic models of water. J. Chem. Phys. 135, 134503 (2011).
[5] Kesselring, T.A., Franzese, G., Buldyrev, S.V., Herrmann, H.J. & Stanley, H.E. Nanoscale Dynamics of Phase Flipping in Water near its Hypothesized Liquid-Liquid Critical Point. Sci. Rep. 2, 474 (2012).
[6] Jeremy C. Palmer, Fausto Martelli, Yang Liu, Roberto Car, Athanassios Z. Panagiotopoulos & Pablo G. Debenedetti, Metastable liquid–liquid transition in a molecular model of water, Nature, 510, 385 (2014).

Competències addicionals[5] (opcional)

Tasques a desenvolupar[6]		**Cronograma** (setmanes)																	
Tasca	**Descripció**	**01**	**02**	**03**	**04**	**05**	**06**	**07**	**08**	**09**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**
T01	**Bibliografia (aprox. 50 h)**	X	X	X	X					X	X	X	X						
T02	**Càlculs preliminars (aprox. 75h)**			X	X	X	X												
T03	**Càlculs etapa 1 (STEP 1) (aprox. 125h)**							X	X	X	X	X	X						
T04	**Càlcul etapa 2 (STEP 2) (aprox. 100h)**										X	X	X	X	X				
T05	**Redacció de la memòria i preparar l'exposició (aprox. 100h)**														X	X	X	X	X
T06																			
T07																			
T08																			
T09																			
T10																			

Observacions i comentaris
Per a la realització del treball pròpiament dit es preveu una dedicació d'unes cinc hores diàries durant cinc dies a la setmana, amb la opció de modificació de l'horari per poder adaptar-se millor a l'horari acadèmic de l'estudiant.

Signatura (el director del TFM)

Signatura (el tutor del TFM, si s'escau)