What ice can teach us about water interactions: a critical comparison of the performance of different water models (1)

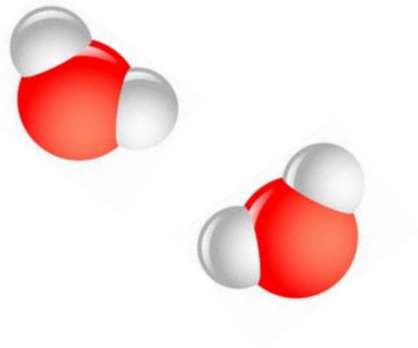
C. Vega, J. L. F. Abascal, M. M. Conde and J. L. Aragones

Facultad de Ciencias Qumicas, Departamento de Quimica Fisica, Universidad Complutense, 28040, Madrid, Spain

• WATER POTENTIAL MODELS

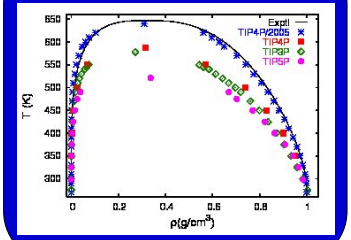
POTENTIAL PARAMETERS

Model	d_{OH}/Å	H-O-H/º	σ/Å	(ε/k_B)/K	q_H/e	d_{OM}/Å	d_{OL}/Å
SPC	1.0	109.47	3.1656	78.20	0.41	0	--
SPC/E	1.0	109.47	3.1656	78.20	0.423	0	--
TIP3P	0.9572	104.52	3.1506	76.54	0.417	0	--
TIP4P	0.9572	104.52	3.1540	78.02	0.52	0.15	--
TIP4P/2005 (2)	0.9572	104.52	3.1589	93.20	0.5564	0.1546	--
TIP5P	0.9572	104.52	3.1200	80.51	0.241	--	0.70

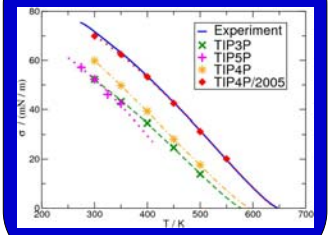


• TESTING THE MODELS FOR TEN PROPERTIES

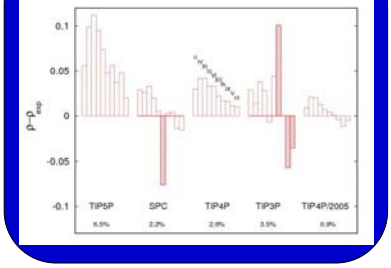
Vapour-liquid equilibria



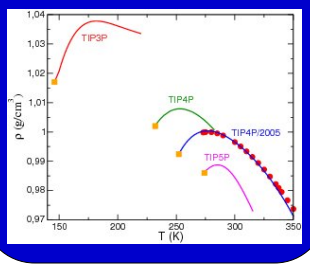
Surface tension



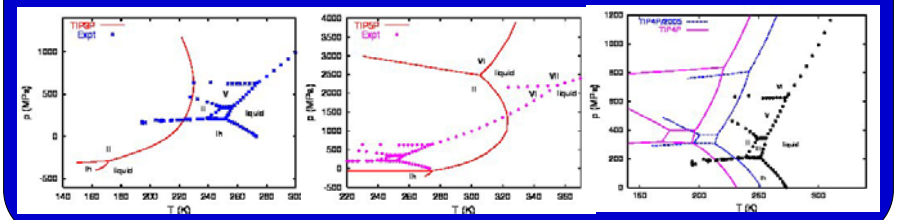
Ice densities predictions



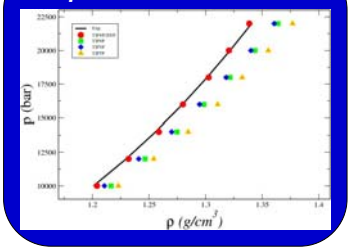
Maximum in density



Phase diagram



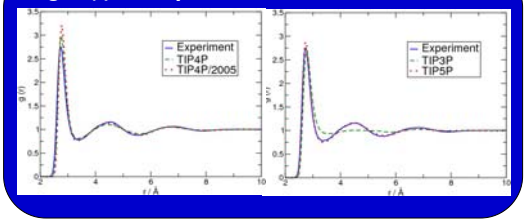
Equation of state T=373K



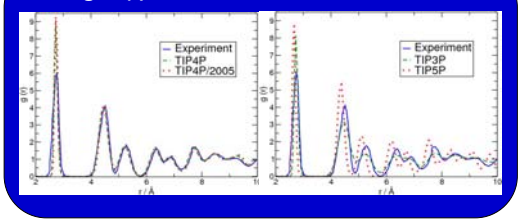
Dielectric const.

Model	ε
TIP3P	94
TIP4P	50
TIP4P/2005	58
TIP5P	91
Experiment	78.4

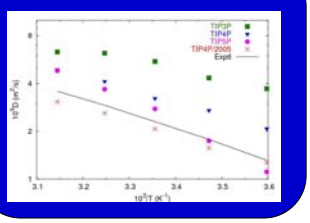
$g_{O\text{-}O}(r)$ for liquid water at 298K and 1bar



$g_{O\text{-}O}(r)$ for ice Ih at 77K and 1bar



Self-diffusion coefficient



• SCORES *(3=the best and 0=the worst)*

Property	TIP3P	TIP4P	TIP4P/2005	TIP5P
1. VLE, T_c	1	2	3	0
2. Surface tension	1	2	3	0
3. ρ Ices	0	2	3	1
4. Phase diagram	0	2	3	1
5. T_m melting prop.	0	1	2.5	2.5
6. T_{TMD}, α, K_T	0	1	3	2
7. Structure	0	1	2.5	2.5
8. EOS (high p)	2	1	3	0
9. D	0	1	3	2
10. ε	2	0	1	3
Total	6	13	27	14

"For most of the properties TIP4P/2005 yields the best performance"

REFERENCES

(1) C. Vega, J.L.F. Abascal, M.M. Conde and J.L. Aragones. *Faraday Discussions* **141** 251-276 (2009)

(2) J.L.F. Abascal and C. Vega. *Journal of Chemical Physics* **123** 234505-1-234505-12 (2005)