

Table of contents

Tuesday 06 October 2015	1
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Workshop on Water at the Interface between Biology, Chemistry, Physics and Materials Sciences | (smr 2707)

Tuesday 06 October 2015

IN-SILICO MODELING OF WATER - LB (Budinich Lecture Hall) (14:00-17:10)

- Conveners: Andrei Tokmakoff / Jeremy Palmer

time	title	presenter
14:00	By chance or by design? Towards a spectroscopically accurate ab-initio water potential from the gas to the condensed phase	FRANCESCO PAESANI
14:40	Ab-initio molecular dynamics of liquid water by quantum Monte Carlo	SANDRO SORELLA
15:20	Coffee break	
15:50	How van-der-Waal's interactions determine the unique properties of water: insights from neural network based simulations	CHRISTOPHER DELLAGO
16:30	The fluid-solid transition in simulation studies of water: thermodynamic and kinetic aspects	CARLOS VEGA DE LAS HERAS