THEO MURPHY INTERNATIONAL SCIENTIFIC MEETING ON

Nanolaboratories: physics and chemistry of small-molecule endofullerenes

Thursday 15 – Friday 16 March 2012

The Kavli Royal Society International Centre, Chicheley Hall, Buckinghamshire

Organised by Professor Malcolm Levitt FRS, Professor Tony Horsewill, Professor Nick Turro and Professor Yas Murata

DAY 1				DAY 2			
09:00	Welcome by Royal Society & Malcolm Levitt /Tony Horsewill			**SESSION 3 Chair: Ron Lawler**		**SESSION 4 Chair: Yasujiro Murata**	
SESSION 1 Chair: Tony Horsewill		**SESSION 2 Chair: Malcolm Levitt**					
09:10	Overview of the spectroscopy of small-molecule endofullerenes **Malcolm Levitt**	**14:00**	Fully coupled quantum calculations of the dynamics and inelastic neutron scattering spectra of a nanoconfined hydrogen molecule: H_2 and HD in C_{60} **Zlatko Bačic**	**09:10**	NMR on endohedral hydrogen in C_{60}-based cages **Marina Carravetta**	**13:45**	Endohedral metallofullerenes – filled fullerene derivatives towards multifunctional reaction center mimics **Dirk Guldi**
09:45	Discussion	**14:35**	Discussion	**09:45**	Discussion	**14:20**	Discussion
10:00	Synthesis and chemistry of small-molecule endofullerenes **Yasujiro Murata**	**14:50**	Inelastic neutron scattering of encapsulated hydrogen molecules in $H_2@C_{60}$: translation-rotation coupling revealed through temperature dependence investigations of time-of-flight spectra **Tony Horsewill**	**10:00**	Photoexcited triplet ENDOR of fullerenes and endofullerenes **John Morton**	**14:35**	Molecular surgical approach to endohedral fullerenes encapsulating He, H_2, and D_2 **Koichi Komatsu**
10:35	Discussion	**15:25**	Discussion	**10:35**	Discussion	**15:10**	Discussion
10:50	Coffee	**15:40**	Tea	**10:50**	Coffee	**15:25**	Tea
11:20	Infrared spectroscopy of small-molecule endofullerenes **Toomas Rõõm**	**16:10**	Motion of fullerene-encapsulated H_2O and H_2 near room temperature: a comparative study by NMR **Ron Lawler and Nick Turro**	**11:20**	Nuclear magnetic resonance studies of endohedral fullerenes: the case of $H_2@C_{70}$ and $H_2O@C_{60}$ **Salvatore Mamone**	**16:10**	Panel Discussion
11:55	Discussion	**16:45**	Discussion	**11:55**	Discussion		
12:10	Predicting NMR relaxation of H_2 in endofullerene nitroxides by DFT calculations **Alessandro Bagno**	**17:00**	Poster session/ general discussion	**12:10**	Poster session/ general discussion	**17:00**	Final remarks **Malcolm Levitt**
12:45	Discussion						
13:00	LUNCH	**19:00**	DINNER	**12:45**	LUNCH	**17:15**	CLOSE