

Oral Programme MC6

Simulation and Theory of Clay Minerals and Interfaces

Convener: Jeffery A. Greathouse, Hendrik Heinz

Thursday 18 June, 2009

Chair: Hendrik Heinz

- 08.50 – 09.20 MC6a.Thu.KL1
*Richard Catlow**
MODELLING OF SILICATE AND ALUMINOSILICATE MATERIALS
- 09.20 – 09.40 MC6a.Thu.L2
James L. Suter, Peter V. Coveney, Mary-Ann Thyveetil, H. Chris Greenwell*
LARGE-SCALE MOLECULAR DYNAMICS REVEALS NOVEL PROPERTIES OF LAYERED NANOMATERIALS
- 09.40 – 10.00 MC6a.Thu.L3
*Artur Meleshyn**
DISTRIBUTION OF MG²⁺, CA²⁺, SR²⁺ AND BA²⁺ AT THE MICA-WATER INTERFACE: A MONTE CARLO STUDY
- 10.00 – 10.20 MC6a.Thu.L4
Jeffery A. Greathouse, Randall T. Cygan*
VIBRATIONAL ANALYSIS OF CLAY MINERALS USING QUANTUM AND CLASSICAL SIMULATIONS

COFFEE BREAK 10.40-11.00

Thursday 18 June, 2009

Chair: Sergey V. Churakov

- 11.00 – 11.30 MC6b.Thu.L1
*Andrey G. Kalinichev**
MULTI-SCALE STRUCTURE AND DYNAMICS OF WATER AT MINERAL SURFACES: MD SIMULATIONS AND EXPERIMENTAL STUDIES
- 11.30 – 11.50 MC6b.Thu.L2
*Hendrik Heinz**
ACCURATE ATOMISTIC SIMULATION OF LAYERED SILICATES AND THEIR INTERFACES
- 11.50 – 12.10 MC6b.Thu.L3
H. Chris Greenwell, Dawn L. Geatches, Peter V. Coveney*
INVESTIGATING ORGANIC – CLAY INTERACTIONS TO UNDERSTAND THE PAST AND SHAPE THE FUTURE
- 12.10 – 12.30 MC6b.Thu.L4
Pavla Capková, Jonáš Tokarský, Kateřina Mamulová Kutláková, Vlastimil Matějka, Marta Valášková*
CLAY MINERALS AS MATRIX FOR FUNCTIONAL NANOSTRUCTURES; MODELING AND EXPERIMENT
- 12.30 – 12.50 MC6b.Thu.L5
Fabrice Salles, Olivier Bildstein, Jean-Marc Douillard, Sabine Devautour-Vinot, Michel Jullien, Henri Van Damme*
DETERMINATION OF THE HYDRATION ENERGY IN SWELLING COMBINING ELECTROSTATIC CALCULATIONS AND EXPERIMENTS

LUNCH 12.50-14.20

Thursday 18 June, 2009

Chair: Andrey G. Kalinichev

- 14.30 – 15.00 MC6c.Thu.L1
*Sergey V. Churakov**
AB INITIO MD SIMULATION OF CLAY MINERALS
- 15.00 – 15.20 MC6c.Thu.L2
*Esther Molina-Montes, Davide Donadio, Alfonso Hernández-Laguna, Michele Parrinello, Ignacio Sainz-Diaz**
DETERMINATION OF THE LIMITING STEP IN THE DEHYDROXYLATION-REHYDROXYLATION REACTIONS IN PYROPHYLLITE BY AB-INITIO MOLECULAR DYNAMIC SIMULATIONS
- 15.20 – 15.40 MC6c.Thu.L3
Raffaella Demichelis, Yves Noel, Philippe D'arco, C. M. Zicovich-Wilson, Roberto Dovesi*
AB INITIO QUANTUM MECHANICAL SIMULATION OF SYSTEMS WITH HELICAL SYMMETRY: CARBON AND CHRYSOTILE NANOTUBES

15.40 – 16.00 MC6c.Thu.L4
*Henryk Wicke**, *Artur Meleshyn*
AB-INITIO AND DENSITY FUNCTIONAL THEORY STUDIES OF HYDRATED SELENITE CLUSTERS

COFFEE BREAK

Thursday 18 June, 2009

Chair: Hendrik Heinz

16.40 – 17.10 MC6d.Thu.L1
*Benjamin Rotenberg**, *Ignacio Pagonabarraga*, *Daan Frenkel*
MESOSOPIC MODELLING OF IONIC DISPERSION AND DIFFUSION IN CLAYS

17.10 – 17.30 MC6d.Thu.L2
*Marie Jardat**, *Jean-François Dufreche*, *Virginie Marry*, *Benjamin Rotenberg*, *Pierre Turq*
COARSE-GRAINING STRATEGY TO STUDY THE SALT EXCLUSION IN MONTMORILLONITE CLAYS

17.30 – 17.50 MC6d.Thu.L3
Ítalo G. Gonçalves, *Carlos O. Petter**, *Paulo Sérgio Criscuolo*, *Milton Luiz Laquintinie Formoso*, *Norberto Dani*
OPTIMIZATION OF BRAZILIAN KAOLIN PROCESSING USING KUBELKA-MUNK THEORY

17.50 – 18.10 MC6d.Thu.L4
*Birthe Klebow**, *Artur Meleshyn*
MONTE CARLO SIMULATION OF QUATERNARY ALKYL AMMONIUM SURFACTANT ADSORPTION ON MUSCOVITE MICA

18.10 – 18.30 MC6d.Thu.L5
*Chandrika Varadachari**
MATHEMATICAL CLASSIFICATION AND GRADING OF CLAY MINERALS

Poster Programme MC6

Posting: Wednesday 17 June, 20.30-22.30. **Removal:** Friday 19 June.

Attendance Time: Thursday 18 June, 18:30–20:00

Chair: Hendrik Heinz

- MC6.Thu.P1 *Petr Kovář**, *Miroslav Pospíšil*, *Zdeněk Futera*, *Kamil Lang*, *Eva Káfuňková*, *Christine Taviot-Guého*, *Petr Bezdička*
ZN-AL LAYERED DOUBLE HYDROXIDE INTERCALATED WITH PORPHYRIN ANIONS; MOLECULAR SIMULATIONS, QM CALCULATIONS AND EXPERIMENTS
- MC6.Thu.P2 *Tiziano Manfredini*, *Monia Montorsi*, *Guido Ori**, *Cristina Siligardi*
MOLECULAR DYNAMICS MODELLING OF HYDRATION AND SWELLING PROCESS OF MONTMORILLONITE
- MC6.Thu.P3 *Miroslav Pospíšil**, *Petr Kovář*, *Pavla Čapková*, *Zdeněk Klik*
MOLECULAR SIMULATIONS OF ORGANIC DYES IN MONTMORILLONITES
- MC6.Thu.P4 *Hiroshi Sakuma**, *Katsuyuki Kawamura*
STRUCTURE AND DYNAMICS OF WATER ON MUSCOVITE MICA SURFACES
- MC6.Thu.P5 *Anton Trník**, *Igor Štubňa*
THERMOMECHANICAL AND THERMODYNAMIC ANALYSIS OF KAOLIN-QUARTZ MIXTURES
- MC6.Thu.P6 *Marek Veteška**, *Miroslav Pospíšil*, *Hana Kostelníková*, *Petr Praus*
NATURAL AND INTERCALATED MONTMORILLONITES ADSORBING PHENOLE AND ANILINE; EXPERIMENT AND MOLECULAR MODELLING
- MC6.Thu.P7 *Tsing-Hai Wang*, *Shih-Min Lin*, *Jiann-Ruey Chen*, *Shi-Ping Teng**
MODELING THE SURFACE ACIDITY OF PHOSPHORIC ACID ACTIVATED MONTMORILLONITE K-10: THE SENSITIVITY ANALYSIS ON SURFACE SITE DENSITY AND DISSOCIATION CONSTANT