



XVII ICC  
ISTANBUL 2022  
25 -29 JULY



## ICC 2022 DETAILED PROGRAM

28 July 2022, Thursday

### TS28 Computational modeling of clays and fluid interfaces

**Convener:** *Kalinichev, A.G., Underwood, T.R.*

- 11:15**     **PHY-1208-Determination of layer charge density by alkylammonium ions: A combined experimental and theoretical assessment of the method**  
*Bruno Lanson, Pierre Mignon, Mélusine Velde, Andreas Bauer, Martine Lanson, Nathaniel Findling, Carlos Perez del Valle*
- 11:30**     **PHY-1289-Classical atomistic simulations of the 10Å phase at high temperatures and pressures**  
*Evgeny Tararushkin, Andrey G. Kalinichev*
- 11:45**     **PHY-1346-Interactions between hydrophobic organic compounds and clay minerals - effect of clay surface charge**  
*Peter Grančič, Leonard Böhm, Martin H. Gerzabek, Daniel Tunega*
- 12:00**     **VRT-1054-From coupling second-order stresses to understanding and predicting the structural response of a dioctahedral smectite**  
*Chadha Mejri, Walid Oueslati, Abdsslem Ben Haj Amara*

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- 14:30**     **PHY-1156-Molecular Dynamics Simulations of the Interaction of Model Petroleum Compounds with Clay Mineral Surfaces**  
*Stanislav R. Stoyanov, Jonathan Y. Manne*
- 14:45**     **PHY-1213-Pore size effects on noble gas uptake in naturally occurring zeolites**  
*Jeffery A. Greathouse, Matthew Paul, Guangping Xu, and Todd R. Zeitler*
- 15:00**     **VRT-1218-Stabilization and organization of water in clay nanotubes**  
*Arianna D'Angelo, Stéphane Rols, Erwan Paineau, Stéphan Rouzière, Viviana Cristiglio & Pascale Launois*