

Contents

Introduction a to special issue on molecular computer simulations of clays and clay–water interfaces: Recent progress, challenges, and opportunities <i>Andrey G. Kalinichev, Xiandong Liu, and Randall T. Cygan</i>	335
Cadmium(II) complexes adsorbed on clay edge surfaces: Insight from first principles molecular dynamics simulation <i>Chi Zhang, Xiandong Liu, Xiancai Lu, Evert Jan Meijer, Kai Wang, Mengjia He, and Rucheng Wang</i>	337
Investigation of the interlayer organization of water and ions in smectite from the combined use of diffraction experiments and molecular simulations. A review of methodology, applications, and perspectives <i>Eric Ferrage</i>	348
Molecular dynamics simulations of anion exclusion in clay interlayer nanopores <i>Christophe Tournassat, Ian C. Bourg, Michael Holmboe, Garrison Sposito, and Carl I. Steefel</i>	374
Molecular simulation of cesium adsorption at the basal surface of phyllosilicate minerals <i>Sebastien Kerisit, Masahiko Okumura, Kevin M. Rosso, and Masahiko Machida</i>	389
Structural and spectroscopic characterization of montmorillonite intercalated with <i>n</i> -butylammonium cations (<i>n</i> = 1–4) – modeling and experimental study <i>Eva Scholtzová, Jana Madejová, L'uboš Jankovič, and Daniel Tunega</i>	401
Stability of the hydronium cation in the structure of illite <i>Elizabeth Escamilla-Roa, Fernando Nieto, and C. Ignacio Sainz-Díaz</i>	413
Effect of polydispersity of clay platelets on the aggregation and mechanical properties of clay at the mesoscale <i>Davoud Ebrahimi, Andrew J. Whittle, and Roland J.-M. Pellenq</i>	425
Comparative computational study of Np(V) and U(VI) adsorption on (110) edge surfaces of montmorillonite <i>Alena Kremleva and Sven Krüger</i>	438
Structure and dynamics of water–smectite interfaces: Hydrogen bonding and the origin of the sharp O–D _w O–H _w infrared band from molecular simulations <i>Marek Szczerba, Artur Kuligiewicz, Arkadiusz Derkowski, Vassilis Gionis, Georgios D. Chryssikos, and Andrey G. Kalinichev</i>	452
Ion adsorption at clay–mineral surfaces: The Hofmeister series for hydrated smectite minerals <i>Thomas Underwood, Valentina Erastova, and H. Chris Greenwell</i>	472
Intercalation of ethylene glycol in smectites: Several molecular simulation models verified by X-ray diffraction data <i>Marek Szczerba and Andrey G. Kalinichev</i>	488
Changes in the interlayer structure and thermodynamics of hydrated montmorillonite under basin conditions: Molecular simulation approaches <i>Jinhong Zhou, Xiancai Lu, and Edo S. Boek</i>	503