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Account No. 20-1402-871

U.S. Nuclear Regulatory Commission
ATTN: Mrs. Deborah A. DeMarco
Two White Flint North
11545 Rockville Pike
Mail Stop T8A23
Washington, DC 20555

Subject: Programmatic Review of Abstract

Dear Mrs. DeMarco:

The enclosed abstract is being submitted for programmatic review. This abstract will be submitted for presentation at the Water-Rock Interactions, to be held June 10–15, 2001, in Sardinia, Italy. The title of this abstract is:

> "Molecular Dynamics Simulation of the Uranyl Ion Near Quartz Surface" by Gregory Bemis, Jeffery Greathouse, and Roberto Pabalan

This abstract is a product of the CNWRA and does not necessarily reflect the view(s) or regulatory position of the NRC.

Please advise me of the results of your programmatic review. Your cooperation in this matter is appreciated.

Sincerely,

Budhi Sagar
Technical Director

BS: ar
d:\gh&gc\fiscal 2000\letters\demarco\20.01402.871 molecular dynamics simulation of the uranyl ion near quartz surfaces
Enclosure

cc:				
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Molecular Dynamics Simulation of the Uranyl Ion Near Quartz Surfaces

Gregory Bemis, Jeffery Greathouse,
Department of Chemistry, St. Lawrence University, Canton, New York, U.S.A.,
and Roberto Pabalan,
Center for Nuclear Waste Regulatory Analyses, 6220 Culebra Road, San Antonio, Texas, U.S.A.

The effectiveness of sorption processes as a mechanism to retard radionuclide migration from nuclear waste repositories depends on the physicochemical characteristics of mineral sorbents and the chemistry of radionuclide-bearing groundwater. Theoretical studies provide a molecular-level description of surface adsorption phenomena that complement experiments. We have used molecular simulation techniques to study the structure and dynamics of an aqueous uranium (VI) species, the uranyl ion, near the quartz (010) surface. Our potential parameters for water, quartz, and other aqueous ions are based on the CVFF forcefield, but for the uranyl ion we used the model of Gilbaud and Wipff (*J. Mol. Struct.* **1996**, *366*, 55) in which uranium carries a charge of +2.5 *e* while each oxygen carries a charge of –0.25 *e*. These partial charges, along with the accompanying short-range potential parameters, produce aqueous uranyl-water and uranyl-carbonate complexes whose geometries are in excellent agreement with available experimental data. Molecular dynamics simulations were performed in the constant NVT ensemble to investigate the ion's sorption characteristics near the quartz surface. Our simulation supercell contains approximately 32 quartz unit cells and 300 water molecules. The adsorbed uranyl ion retains a five-fold solvation shell, while the O–U–O axis aligns perpendicular to a surface with singly protonated sorption sites.

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