

Molecular Dynamics Studies of Small Molecule Adsorption on Iron Oxide

Thursday 10 July 2025 16:15 (20 minutes)

High-temperature corrosion protection of low-alloy steel in steam generators of nuclear power plants is provided by a layer of magnetite. The presence of various small molecules in the cooling system affects the flow-assisted corrosion processes. The molecular dynamics (MD) method allows for an in-depth analysis of the mechanism and extent of adsorption of such molecules on magnetite at the molecular level. In the present work, a model surface {111} of magnetite with a layer thickness of 2.50 nm and a side length of 3.39 nm is constructed. The incorporation of such a complex system into MD simulation requires a modification in the imposed molecular mechanical force field (Clay FF). Two model systems consisting of a magnetite surface in the presence of an aqueous medium with ammonia or ethanolamine molecules are considered. MD calculations were performed in the NPT ensemble at a pressure of 90 bar using the TIP3P water model. For the two systems, different temperature ranges are simulated –for ammonia the temperature range is up to 473 K [1], for ethanolamine it is up to 503K. Data on the extent of adsorption have been obtained, the root mean square deviation (RMSD) of the target molecules has been calculated and their minimum distance to the magnetite surface has been traced. A comparison has been made with existing experimental results [2] and similar MD simulations.

References:

- 1 N. Ivanova, V. Karastoyanov, I. Betova, M. Bojinov, *Molecules*, 29, 3276 (2024).
- 2 M. Bojinov, I. Betova, N. Ivanova, V. Karastoyanov, *Materials*, 18, 944 (2025).

Acknowledgment: This study is funded by the European Union-NextGenerationEU, through the National Recovery and Resilience Plan of the Republic of Bulgaria, project № BG-RRP-2.004-0002 (BiOrgaMCT).

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Session Classification: Condensed Matter, Materials and Applied Physics

Track Classification: S03 –Condensed matter, Materials and Applied Physics