化生研 講演会/ CLS Seminar

Institute of SCIENCE TOKYO

Photoelectrochemical water splitting on hematite: Mechanistic insights from atomic-scale modeling

Lecturer: **Dr. Simone Piccinin**
National Research Council
Trieste, Italy

Time & Date: 15:30-17:00, Monday 29 Sept 2025

Place: The 3rd Seminar Room, R1 bldg. Suzukakedai campus
(R1棟2F 第三会議室)

Abstract: The oxygen evolution reaction (OER) plays a crucial role in (photo)electrochemical devices that use renewable energy to produce synthetic fuels. Recent measurements on semiconducting oxides have shown that the dependence of the rate of OER on the surface hole density is a power law, suggesting a multihole mechanism. We have used machine learning interatomic potentials to model this process in hematite, Fe_2O_3. We find that the reaction proceeds via direct coupling of oxygen adsorbates. Using microkinetic modeling, we find that the rate vs hole coverage has a third order dependence, driven by facile formation of the superoxo intermediate, a step whose barrier is weakly dependent on the surface hole coverage.

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