

DEPARTMENTAL SEMINAR Condensed Matter and Materials Physics

31st January, 2023

4.00 PM

ONLINE/ FERMION

SPEAKER

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TITLE OF THE TALK

DYNAMICS OF H20 DISSOCIATION ON METAL SURFACES

ABSTRACT

Dissociation of H2O on a metal surface is rate-limiting step in many industrially important reactions. In a few recent experiments, it has been observed that dissociation of H2O on a metal surface is mode-selective. In other words, this reaction is not statistical in nature and therefore, one cannot use transition state-based theories to get insights of this reaction. Our quantum dynamical calculations show that mode-mode coupling along the reaction path is the key factor in deciding the quantum of mode-selectivity in this reaction.

HOST FACULTY

Prof. Manoranjan Kumar, Professor
