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Diffusion on Cu Surface under Electric Field with Collective Variable -accelerated Molecular Dynamics

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Atomic diffusion on metallic surfaces under electric field is known to be biased towards higher field values. In the vicinity of a field-enhancing protrusion, stochastically hopping surface atoms are hypothesized to contribute to the growth of the protrusion by this bias mechanism.

In the context of the Compact Linear Collider (CLIC), field-enhancer growth by diffusion is one of the mechanisms proposed to play a role in the build-up of electrical breakdowns that disrupt the operation of the collider. The events immediately preceding a breakdown are difficult to observe experimentally, and thus simulation methods can often greatly assist in the study of these phenomena.

In this work, we have studied the Cu surface under electric field by Molecular Dynamics (MD). The electric field is implemented with the Femocs library [1]. To overcome the timescale limitation of MD, we have used Collective Variable -driven Hyperdynamics (CVHD) acceleration [2]. This way, the long timescale diffusion events can be simulated more efficiently.

In this presentation, we will give a short overview of the methodology, and discuss the results of our work in progress.

[1] Veske, Mihkel, et al. Journal of Computational Physics 367 (2018): 279-294.

[2] Bal, Kristof M., and Erik C. Neyts. Journal of chemical theory and computation 11.10 (2015): 4545-4554.

Authors: KIMARI, Jyri; DJURABEKOVA, Flyura (University of Helsinki)

Presenter: KIMARI, Jyri

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