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Molecular simulations in electrochemistry

Electron and proton transfer reactions mediated by flavins in different molecular environments

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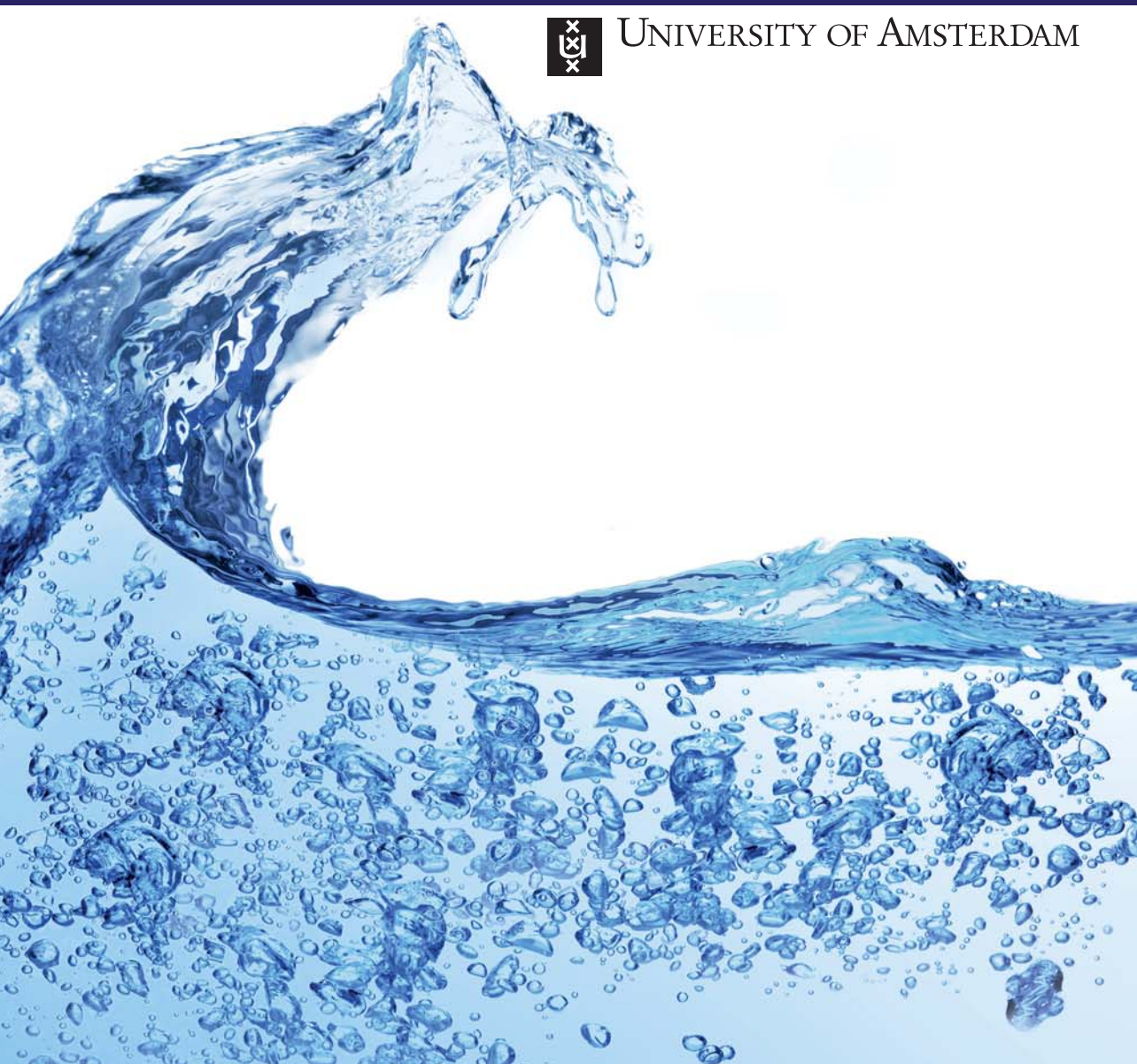
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Protons and electrons are very light particles that can move with a high velocity, but in practice their transfer is strongly affected by the medium. The conductivity is governed by the solvent fluctuations.

Confinement of the solvent in one or more dimensions affects the transfer mechanism. The solvent reorganization free energy is an important part of both the redox potential and the acidity constants of acceptor solutes.



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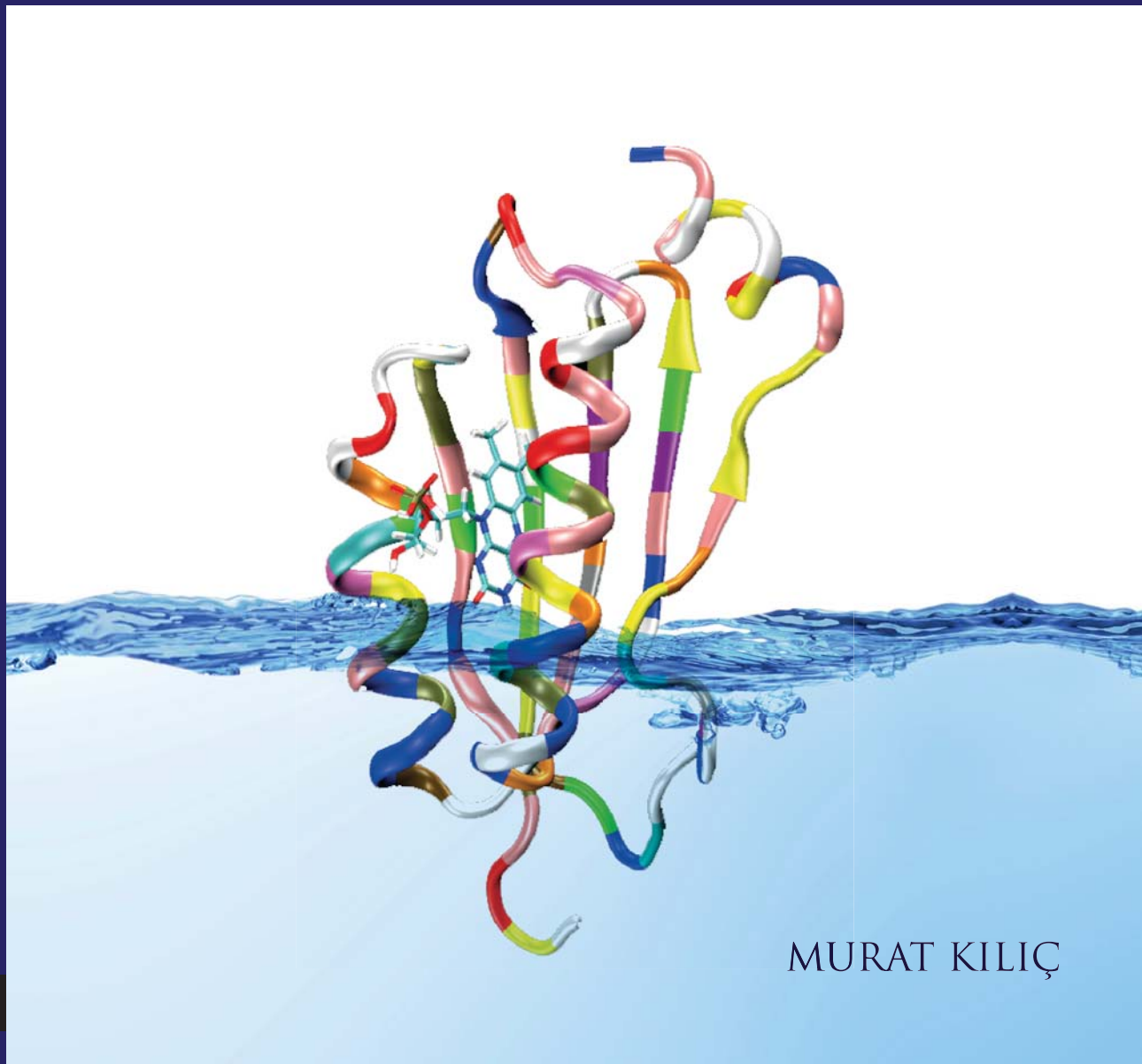
MURAT KILIÇ

MOLECULAR SIMULATIONS IN ELECTROCHEMISTRY



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