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Computational electrocatalysis: methods and fundamental applications on CO₂ reduction and formic acid oxidation

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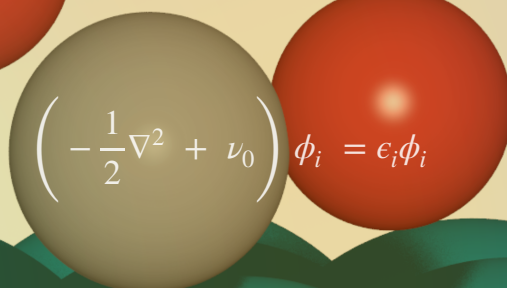
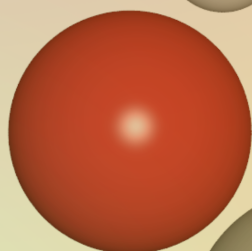
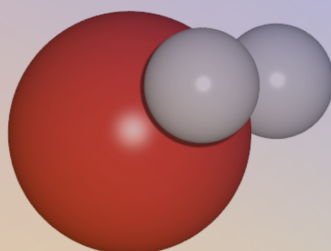
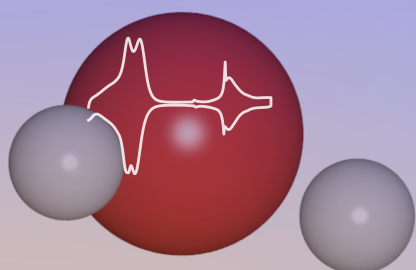
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COMPUTATIONAL ELECTROCATALYSIS: METHODS AND FUNDAMENTAL APPLICATIONS ON CO₂ REDUCTION AND FORMIC ACID OXIDATION

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$$\left(-\frac{1}{2}\nabla^2 + \nu_0 \right) \phi_i = \epsilon_i \phi_i$$

