Molecular simulations in electrochemistry

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

1 Introduction 1
  1-1 Electron transfer in chemistry ........................................ 2
  1-2 Proton transfer in chemistry ........................................... 3
  1-3 Flavins in chemistry ................................................... 4
  1-4 Molecular simulation .................................................. 5
  1-5 Model and methods ..................................................... 5
  1-6 This thesis ............................................................. 6

2 Techniques 9
  2-1 Marcus theory .......................................................... 10
  2-2 Calculation of $pK_a$ using molecular simulation ................. 13
  2-3 Statistical thermodynamics ........................................... 15
  2-4 Molecular dynamics .................................................. 16
  2-5 DFT–based molecular dynamics ...................................... 17
    2-5.1 Density Functional Theory ....................................... 19
    2-5.2 Born–Oppenheimer molecular dynamics ......................... 21
  2-6 Hybrid quantum mechanics / molecular mechanics ............... 22

3 First and second one-electron reduction of lumiflavin in water – a
   first principles molecular dynamics study 23
  3-1 Introduction .......................................................... 24
  3-2 Methods .............................................................. 25
    3-2.1 Computational setup .............................................. 29
  3-3 Results ............................................................... 30
    3-3.1 Lumiflavin in the gas phase .................................... 30
    3-3.2 Lumiflavin in water, the solvent structure .................... 33
    3-3.3 Lumiflavin in water, redox properties .......................... 39
    3-3.4 Non–linearity, inner sphere fluctuations, temperature and finite
         size effects ......................................................... 41
  3-4 Conclusions ........................................................... 44
  3-5 Supporting information ............................................... 46
A microscopic picture of the solvent reorganization during electron transfer to flavin in water

4-1 Introduction ....................................................... 51
4-2 Methods .......................................................... 52
  4-2.1 Calculation of redox potential .............................. 52
  4-2.2 Computational setup ....................................... 54
4-3 Results .......................................................... 56
  4-3.1 Reduction of lumiflavin in vacuum ......................... 56
  4-3.2 Reduction of lumiflavin in water solvent .................. 58
  4-3.3 Inner sphere and solvent reorganization, solvation shell structure rearrangement .......... 60
  4-3.4 Solvent reorganization, electronic effects ................. 62
  4-3.5 Solvent reorganization, electrostatic potential and fluctuations .................. 64
4-4 Conclusions .................................................... 66
4-5 Appendix ....................................................... 70

Acidity constants of lumiflavin from first principles molecular dynamics simulations

5-1 Introduction ....................................................... 71
5-2 Methods .......................................................... 72
  5-2.1 Calculation of pKₐ from constrained dynamics .......... 72
  5-2.2 Computational details ..................................... 74
5-3 Results and discussion ........................................ 76
5-4 Conclusions .................................................... 78
5-5 Supplementary information .................................... 80
  5-5.1 Radial distribution functions .............................. 80
  5-5.2 Free energy profiles using the addition H₃O⁺ restraint .......... 82

The reorganization free energies for electron transfer in proteins: Redox properties of flavin in BLUF and LOV Domains

6-1 Introduction ....................................................... 91
6-2 Methods .......................................................... 92
  6-2.1 Computational setup ....................................... 92
6-3 Results .......................................................... 94
  6-3.1 Reduction of flavin in different environments .......... 94
  6-3.2 Characterization of protein and solvent coupling with flavin redox properties ............. 96
6-4 Conclusions .................................................... 98

Summary .......................................................... 100

Samenvatting ...................................................... 102