Excited-state solvation structure of transition metal complexes from molecular dynamics simulations and assessment of partial atomic charge methods - DTU Orbit (04/03/2019)

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In this work, we investigate the excited-state solute and solvation structure of [Ru(bpy)_3]^{2+}, [Fe(bpy)_3]^{2+}, [Fe(bmip)_2]^{2+} and [Cu(phen)]^{2+} (bpy = 2,2'-bipyridine; bmip = 2,6-bis(3-methyl-imidazole-1-ylidine)-pyridine; phen = 1,10-phenanthroline) transition metal complexes (TMCs) in terms of solute-solvent radial distribution functions (RDFs) and evaluate the performance of some of the most popular partial atomic charge (PAC) methods for obtaining these RDFs by molecular dynamics (MD) simulations. To this end, we compare classical MD of a frozen solute in water and acetonitrile (ACN) with quantum mechanics/molecular mechanics Born-Oppenheimer molecular dynamics (QM/MM BOMD) simulations. The calculated RDFs show that the choice of a suitable PAC method is dependent on the coordination number of the metal, denticity of the ligands, and type of solvent. It is found that this selection is less sensitive for water than ACN. Furthermore, a careful choice of the PAC method should be considered for TMCs that exhibit a free direct coordination site, such as [Cu(phen)]^{2+}. The results of this work show that fast classical MD simulations with ChelpG/RESP or CM5 PACs can produce RDFs close to those obtained by QM/MM MD and thus, provide reliable solvation structures of TMCs to be used, e.g. in the analysis of scattering data.

General information
State: Published
Organisations: Department of Chemistry, Department of Physics
Number of pages: 14
Pages: 4082-4095
Publication date: 2019
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 21
Issue number: 7
ISSN (Print): 1463-9076
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.04 SJR 1.686 SNIP 1.089
Web of Science (2017): Impact factor 3.906
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.06 SJR 1.685 SNIP 1.113
Web of Science (2016): Impact factor 4.123
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.45 SJR 1.725 SNIP 1.205
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.29 SJR 1.771 SNIP 1.239
Web of Science (2014): Impact factor 4.493
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 4.05 SJR 1.72 SNIP 1.207
Web of Science (2013): Impact factor 4.198
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.67 SJR 1.921 SNIP 1.177