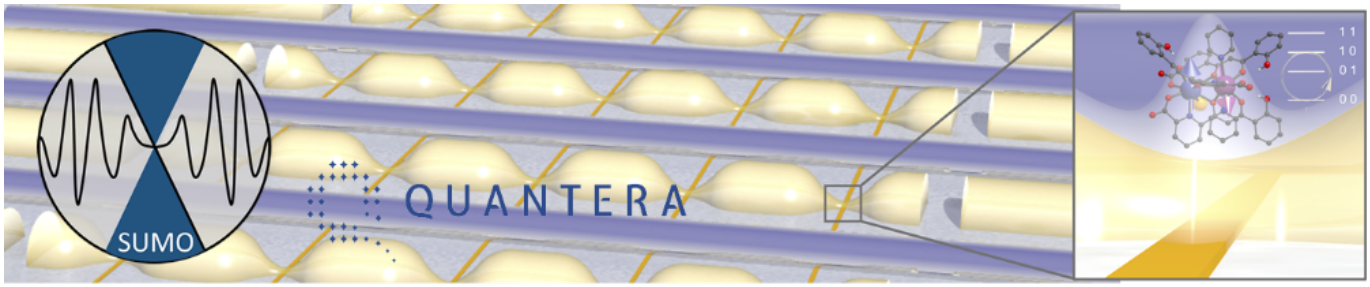

Open data management. Description of available data and metadata related to a publication	
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Date	2019/05/01
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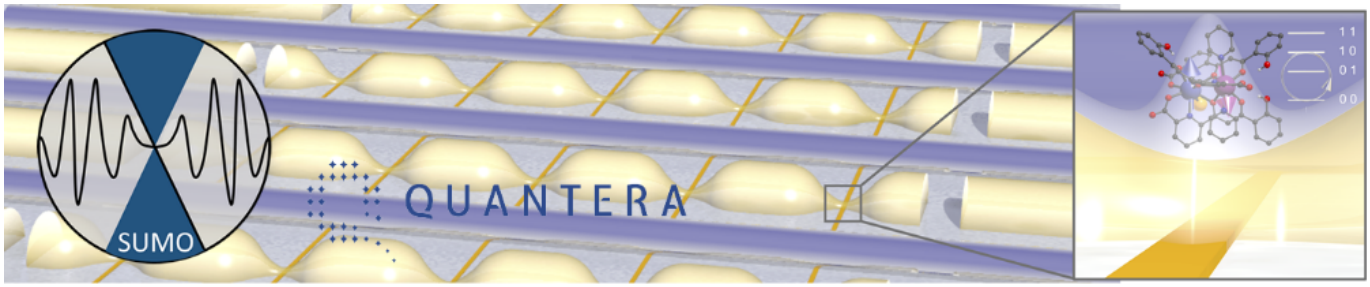
Paper citation	Physical Chemistry Chemical Physics, **21**, 10908-10913 (2019)
Language	English
Dataset ID	SUMO_ICMol_Rosaleny_2019_01
List of data files available	*c9cp01909j1.pdf* *c9cp01909j2.zip (amberhack2simpre.py, hack_atoms.f90, makefile, path.txt, pmemd.f90, runmd.f90)*
Methodology	*Implementation of the first in silico exploration of the explicit time-dependent dynamics of spin energy levels due to thermal molecular movements, employing force fields. We combined two inexpensive computational tools, namely molecular dynamics (MD) as implemented in the Amber2017 package and crystal field modelling based on effective point charges as implemented in the SIMPRE software to extract the energies of the 13 MJ states of the J = 6 ground multiplet at different times. The studied system was a family of peptides known as Lanthanide Binding Tags (LBTs).*
Data processing and software needed	*Details of MD and spin energy level calculations, B3LYP and RPMD results, Fortran & Python scripts, and autocorrelation and fast Fourier transform plots*
Access to the data	As files in the Electronic Supplementary Information via the journal website: https://pubs.rsc.org/en/content/articlelanding/2019/cp/c9cp01909j


SUMO
QUANTERA
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