Computational Study of macrocyclic crown thio ethers

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Crown thioethers are organic molecules that can act as molecular, metal and radioisotope carriers, ion-sensitive electrodes, phase transfer reagents and etc [1]. When these lock and key compounds are functionalized with radioisotopes, they present promising possibilities to be applied in drug design to treat and diagnose diseases. The Time Differential Perturbed Angular Correlation (TDPAC) technique has been suggested in the literature, in connection with different radioactive probes, to aid in this study [2,3]. An important issue to be addressed in the case of biomedical applications is the structural stability of the Crown thioethers, under different conditions, what can be done through state of the art *ab initio* electronic structure calculations. Here we study the electronic, structural and electrical hyperfine properties of some Crown thioethers complexed with Ag or Cd. We try to reproduce the different situations faced when there is a β decay of ^{111}Ag to ^{111}Cd as seen in a TDPAC experiment. We use the CP-PAW code, which is an all electron *ab initio* method in the Kohn-Sham scheme of the DFT [4] combining the Car-Parrinello quantum molecular dynamics [5] and the Projector Augmented Wave basis (PAW) set [6]. Our Electric Field Gradient (EFG) results are in a very good agreement with measurements [7] when the Cd+ atom is used to mimic the experimental situation. We also discuss the similarity in the electronic structures before and after the decay. We demonstrate in this issue the importance to evaluate the correct charge state in the *ab initio* analysis.

References

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