

# f-ELEMENT SERIES COLOGNE

## THEORETICAL ACTINIDE MOLECULAR SCIENCE



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### Georg in 3 sentences

THE FASCINATION OF F-ELEMENTS FOR ME IS FOUND IN THE UNIQUE CHEMISTRY OF THE ACTINIDES, INCLUDING SUBTLE CHANGE FROM ONE ELEMENT TO THE NEXT.

MY FAVOURITE PUBLICATION... WELL, THAT'S A TOUGH ONE!!!

MY BIGGEST MOTIVATION:  
MY STUDENTS AND MY FAMILY, AS WELL AS CURIOSITY ("ZU ERKENNEN WAS DIE WELT IM INNERSTEN ZUSAMMENHÄLT").

*Computational actinide chemistry* is the application of the tools of computational chemistry to the actinides. We will begin by discussing some aspects of the computational methodology, and then focus on selected applications; specifically, (i) molecular calculations: complexes with macrocycles, including crown ethers and the famous 'pacman' ligand; (ii) mineral surface interactions: adsorption of uranyl species onto  $\text{TiO}_2$  surfaces; (iii) interactions of actinides with 2D materials. We will attempt to draw specific as well as general conclusions regarding methodology and the chemistry involved. Thus, we hope to illustrate the scope of questions that can be addressed, and the kind of unique insight that computational chemistry might provide.

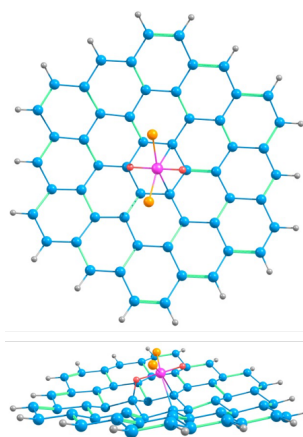


Fig. 1: Interaction of uranyl with silicene (2D Si); top and side view of optimized structure.

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HÖRSAAL III

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