WG4 – How the different cathodic metals perturb the CF_3^+ potential energy curves

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Activities

To be able to cope with a problem of electrode aging we want to use quantum-chemical calculation to get deeper insight into the processes on electrodes
In regard to that we constructed Potential Energy Surface (**PES**) in vicinity of boundary phase of cathode composed of different metals for CF_3^+ ion which appear in plasma during gaseous detector use.
Using quantum chemical calculations, DFT method and appropriate basis set we construct **PES**

We optimize structures for minimum energy for CF_3^+ ion for chosen distance from electrode – cathode with different metal surface and record their energies
We simulated Cu, Ag, Au and Al electrode for CF_3^+ ion, which we previously optimized and hold fixed during simulations

Motivation

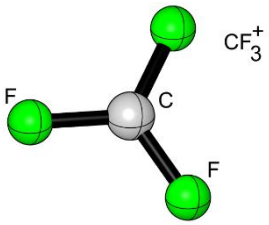
In spite we have knowledge about reaction in bulk, i.e. plasma,
electrodes can on different way perturb energetic levels of our investigated ion
so we need to enlarge out knowledge in way in which electrodes perturb
bonds in our ion which lead to stabilization or destabilization

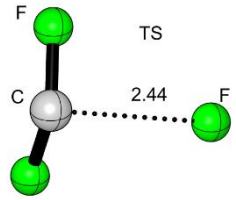
Degradation pathway of CF_3^+ in bulk, in plasma

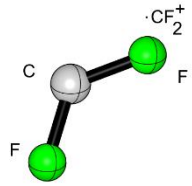
$CF_3^+ \rightarrow \cdot CF_2^+ + \cdot F$ (R1) E_a=7.11 eV

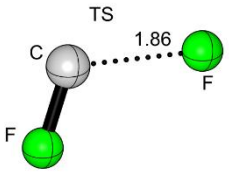
$\cdot CF_2^+ \rightarrow CF^+ + \cdot F$ (R2) E_a=3.63 eV

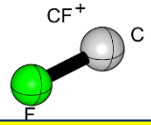
$CF^+ \rightarrow \cdot C^+ + \cdot F$ (R3) E_a=9.36 eV

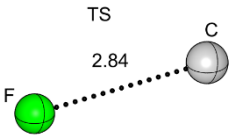






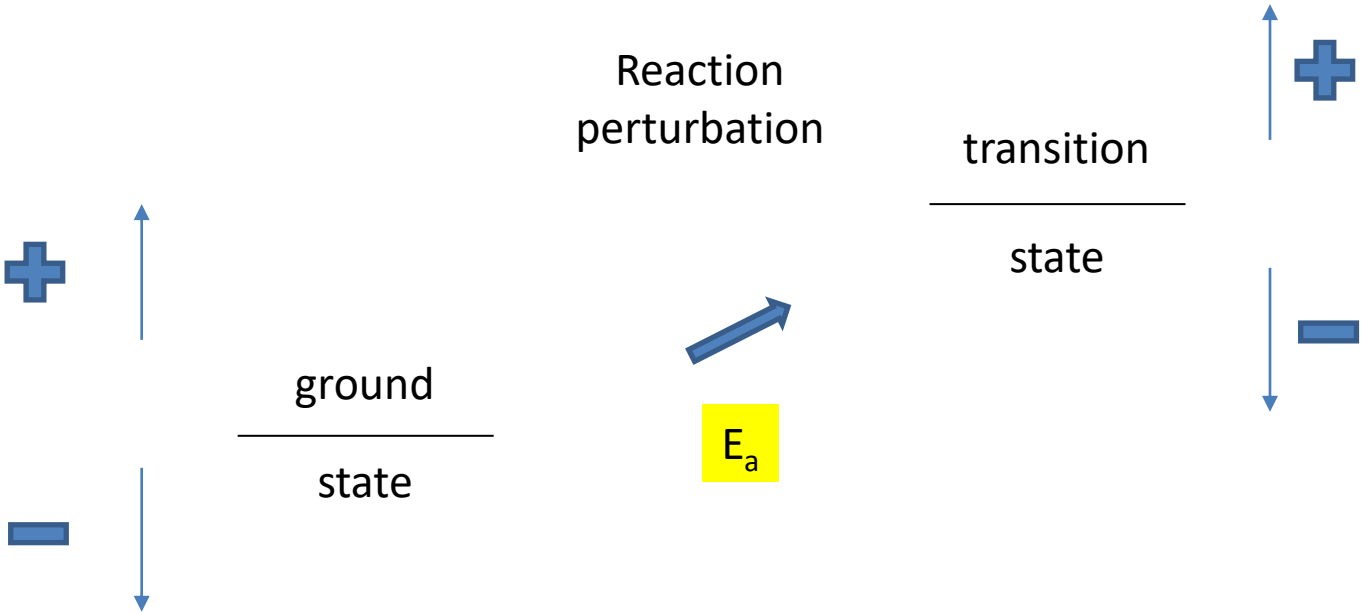






Ground state

Transition state



Near the electrode surface energy levels of ion can be stabilized or destabilize in ground and also in transition state

In order to investigate perturbation we calculate Potential Energy Surface for CF_3^+ ion approaching electrode of different metals:

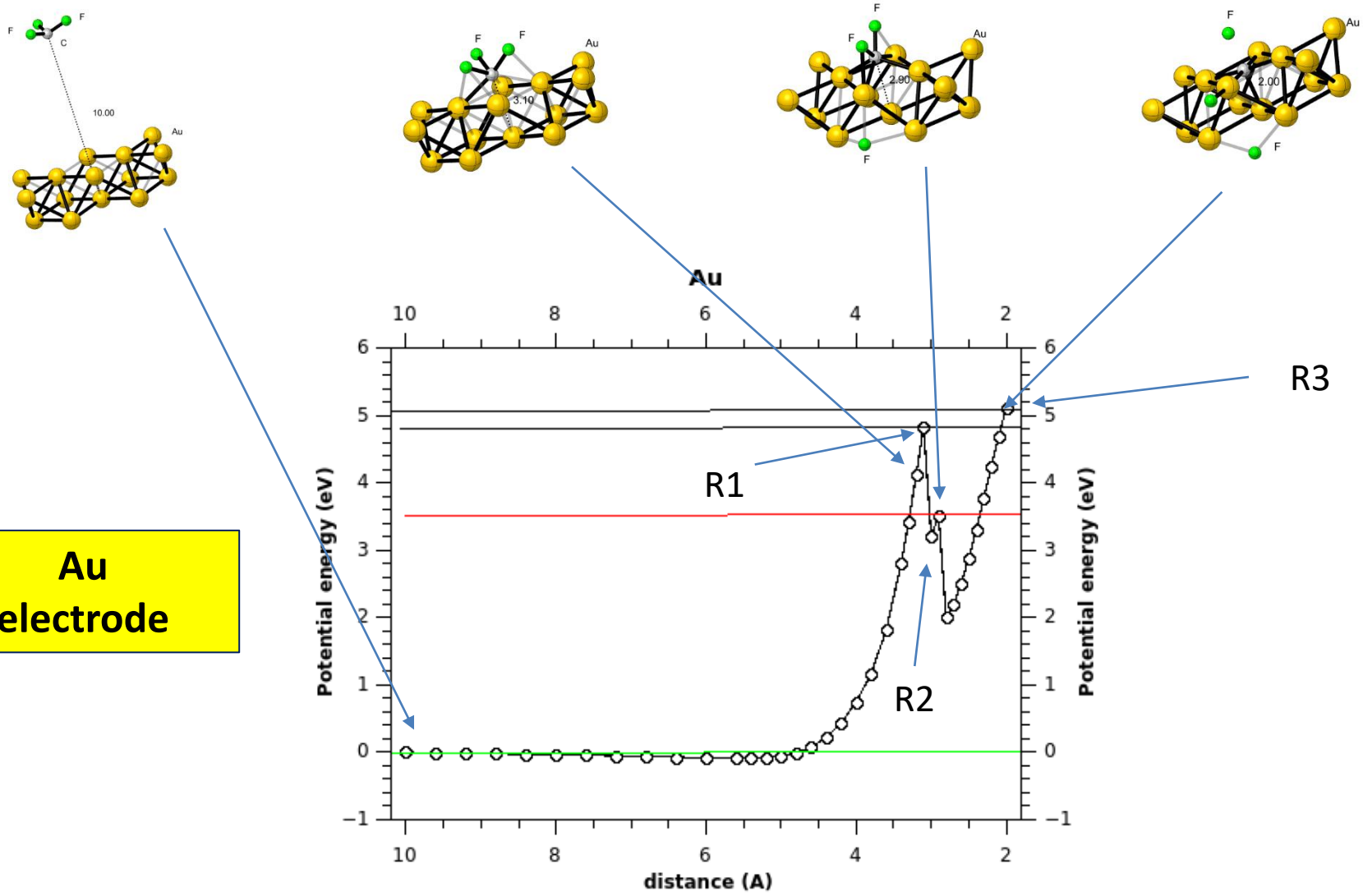
Au

Ag

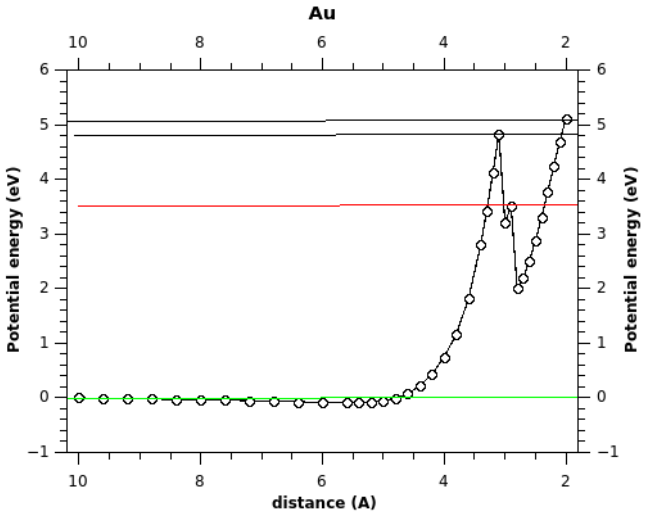
Cu

Al

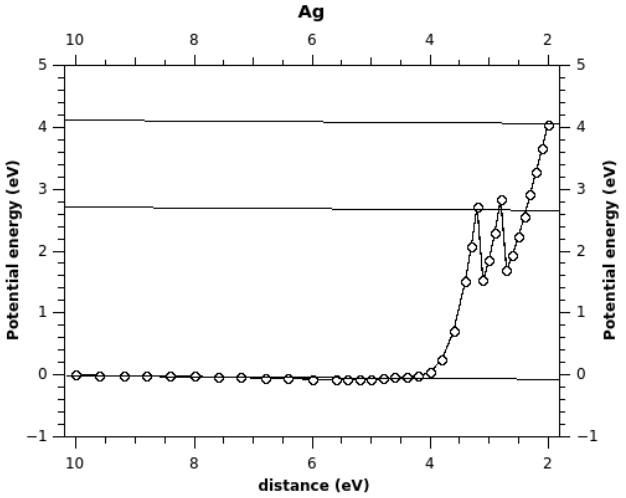
Quantum chemical calculation were performed with ORCA and gaussian package at different theoretical level and appropriate basis set



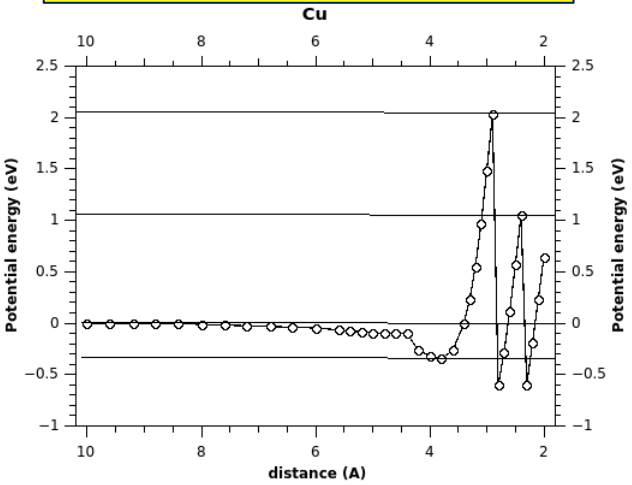
Au electrode



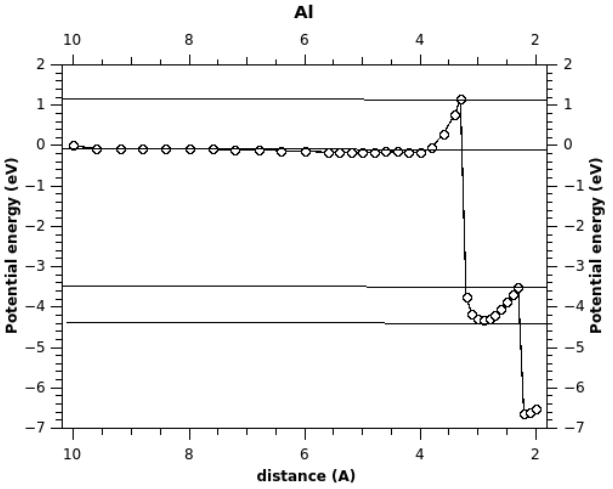
PES for Au electrode



PES for Ag electrode

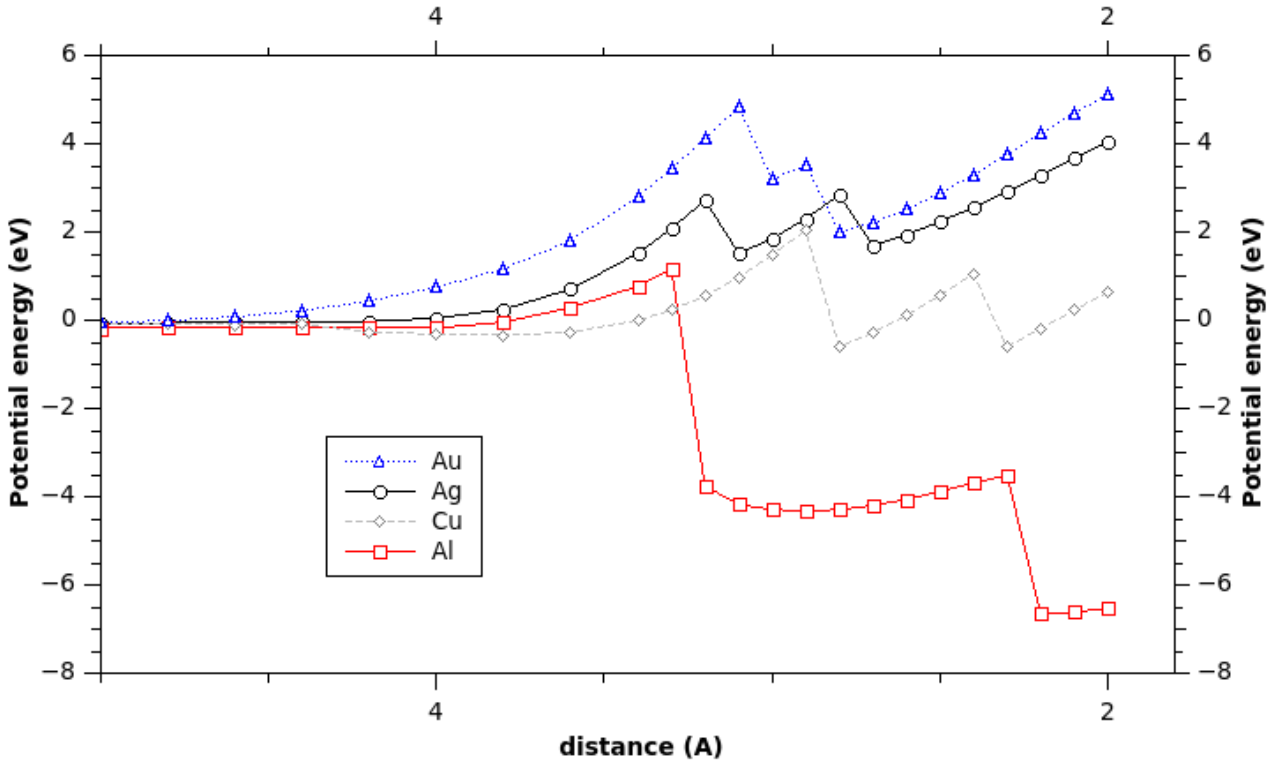


PES for Cu electrode



PES for Al electrode

Comparison of PES for different electrode metals



Conclusion

- **To the best of our knowledge this is the first time of such investigation.**
- **PES for different electrodes metal show different behavior.**

DRD1 Future Plans

Longevity and aging

- Construction of Potential energy surface (PES) in vicinity of boundary phase for both electrodes b y using quantum chemical calculations for eco-friendly gases
- Construction of Potential energy surface (PES) in vicinity of boundary phase for both electrodes by using quantum chemical calculations for eco-friendly gases with different electrodes materials