XXXIX REUNIÓN
BIENAL DE QUÍMICA
Zaragoza 2023

25 - 29 de junio
Auditorio de Zaragoza
www.bqz2023.com

COMPUTATIONAL INSIGHT INTO HYBRID ORGANIC-METAL INTERFACES WITH BIOSENSING PROPERTIES

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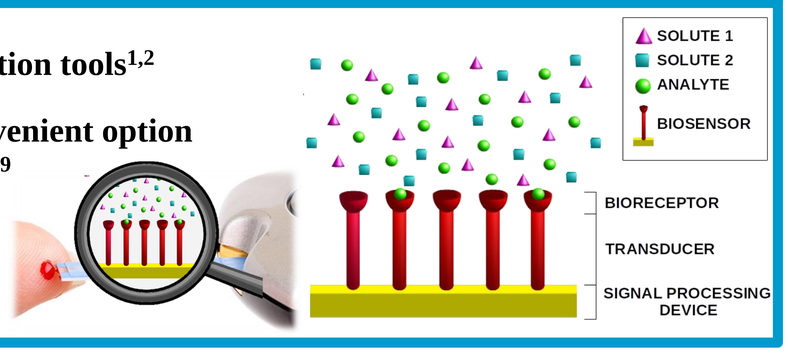
MoBioChem – Modeling Biology and Chemistry

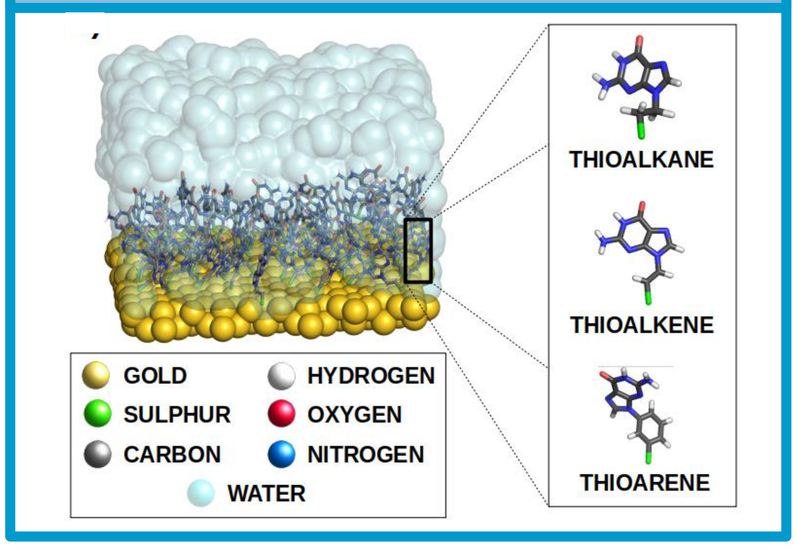
MoI-PM – Molecular Processes Modeling Group

MOTIVATION

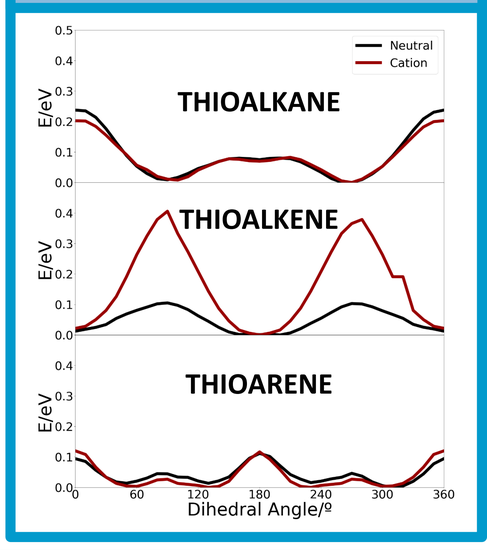
- Biosensors are powerful detection tools[1,2]
- DNA-based biosensors as convenient option for electrochemical detection[3-9]
- Redox properties near the interface are unknown



SYSTEM

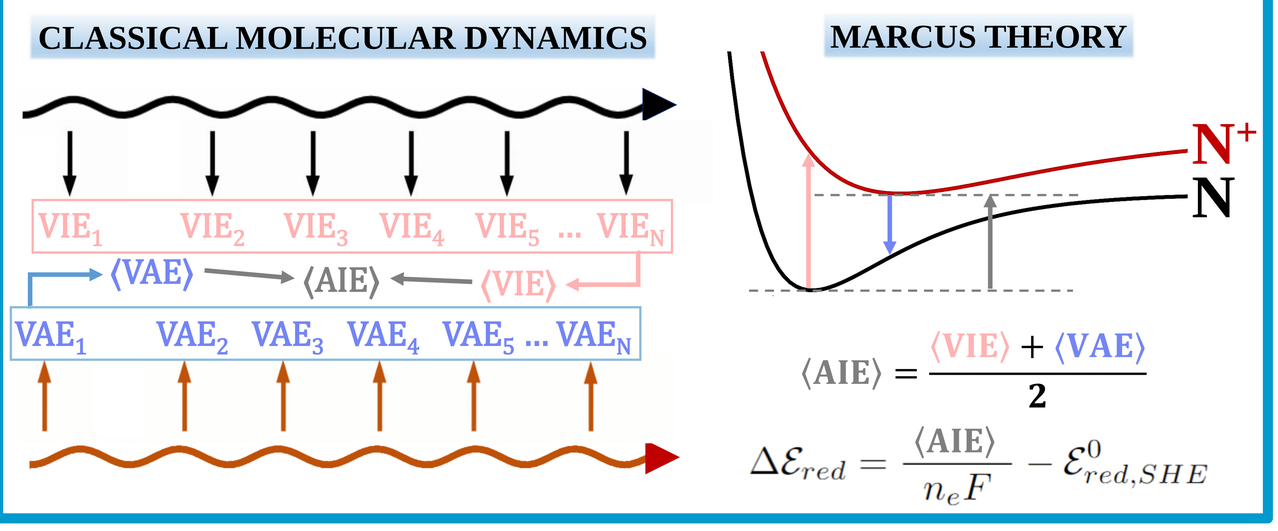


SCAN



MD WITHIN MARCUS THEORY

$$N^+_{(aq)} + e^-_{(gas)} \xrightarrow{AIE} N_{(aq)}$$

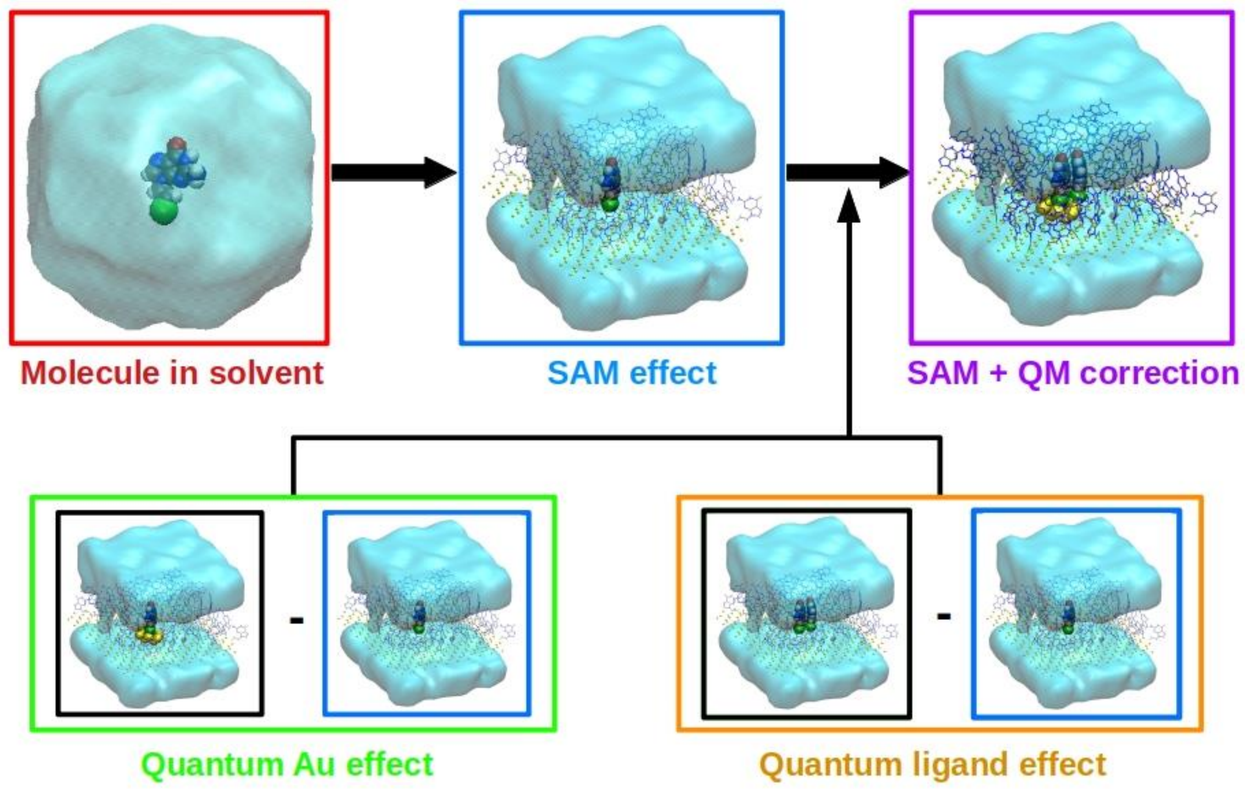


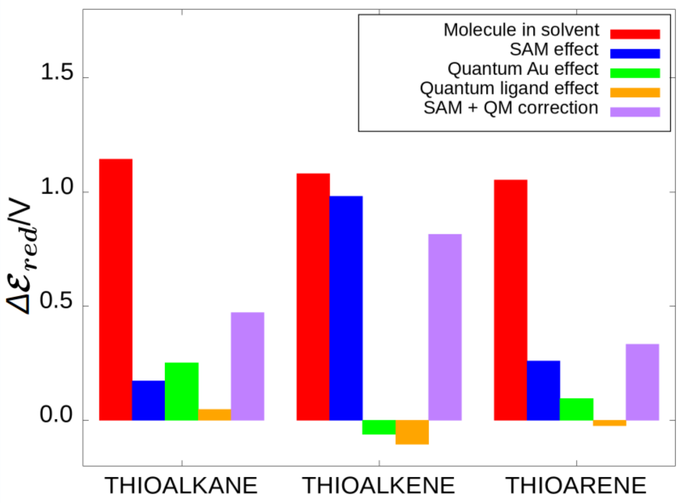
$$\langle AIE \rangle = \frac{\langle VIE \rangle + \langle VAE \rangle}{2}$$

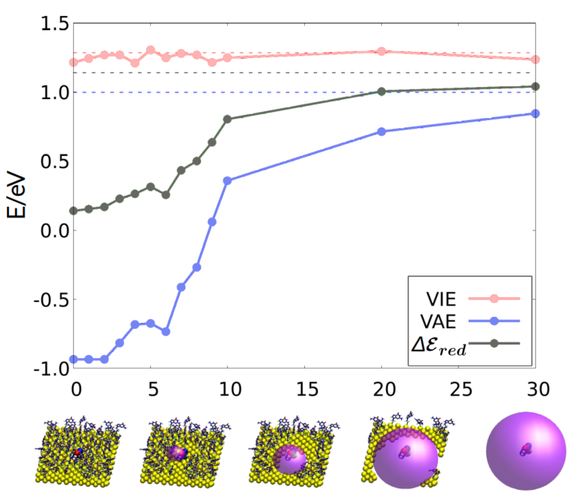
$$\Delta\mathcal{E}_{red} = \frac{\langle AIE \rangle}{n_e F} - \mathcal{E}^0_{red,SHE}$$

ADDITIVE SCHEME

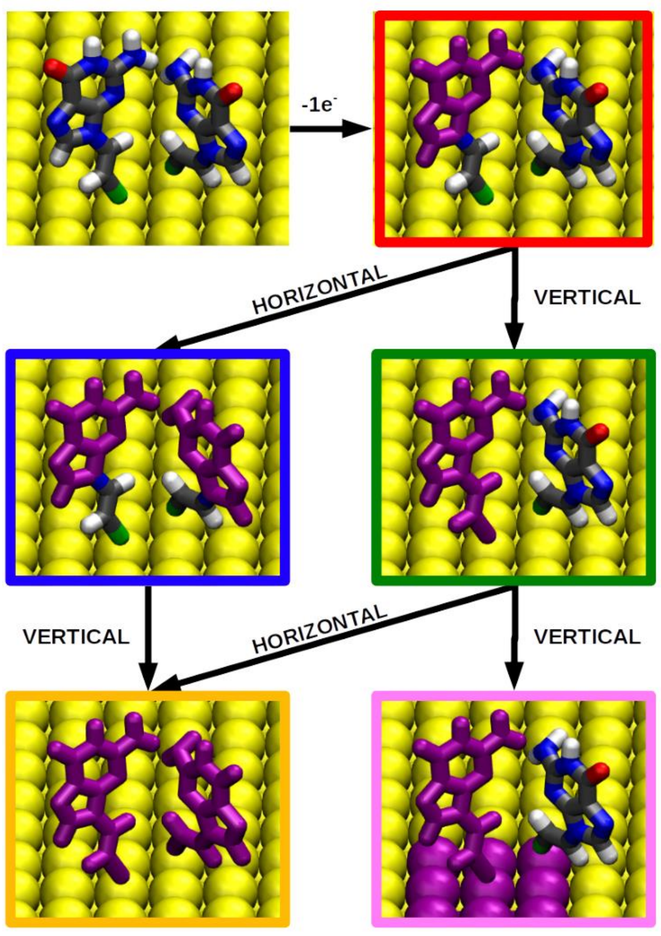
$$\Delta\mathcal{E}_{red,2L-4Au} = \Delta\mathcal{E}_{red,1L} + (\Delta\mathcal{E}_{red,1L-4Au} - \Delta\mathcal{E}_{red,1L}) + (\Delta\mathcal{E}_{red,2L} - \Delta\mathcal{E}_{red,1L})$$

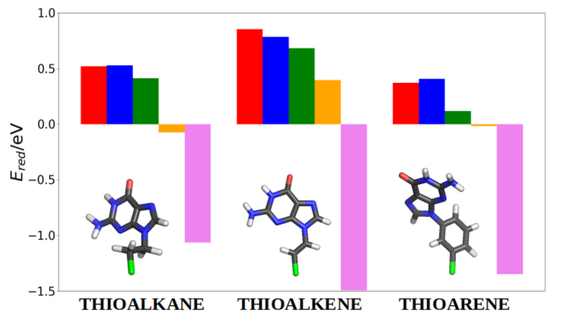


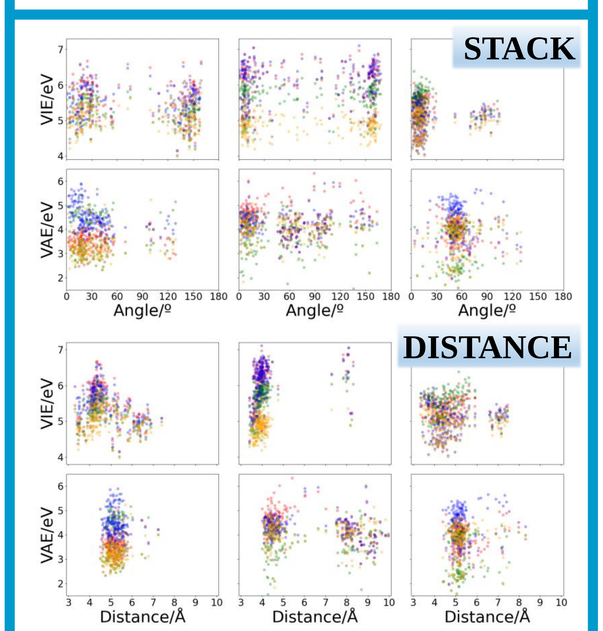




MOST PROBABLE PATHWAY







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CONCLUSIONS

- Reducer character of guanine increases when going from aqueous phase to a SAM due to electrostatic interactions with other neighbour ligands.
- Reducer character can be tuned changing the nature of linker in a SAM.
- A hole will likely migrate from the ligand to the surface vertically with extra stabilization of the electrostatic interactions with other ligands.

IAdChem – Institute for Advanced Research in Chemistry
RES – Red Española de Supercomputación
UAM – Universidad Autónoma de Madrid
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