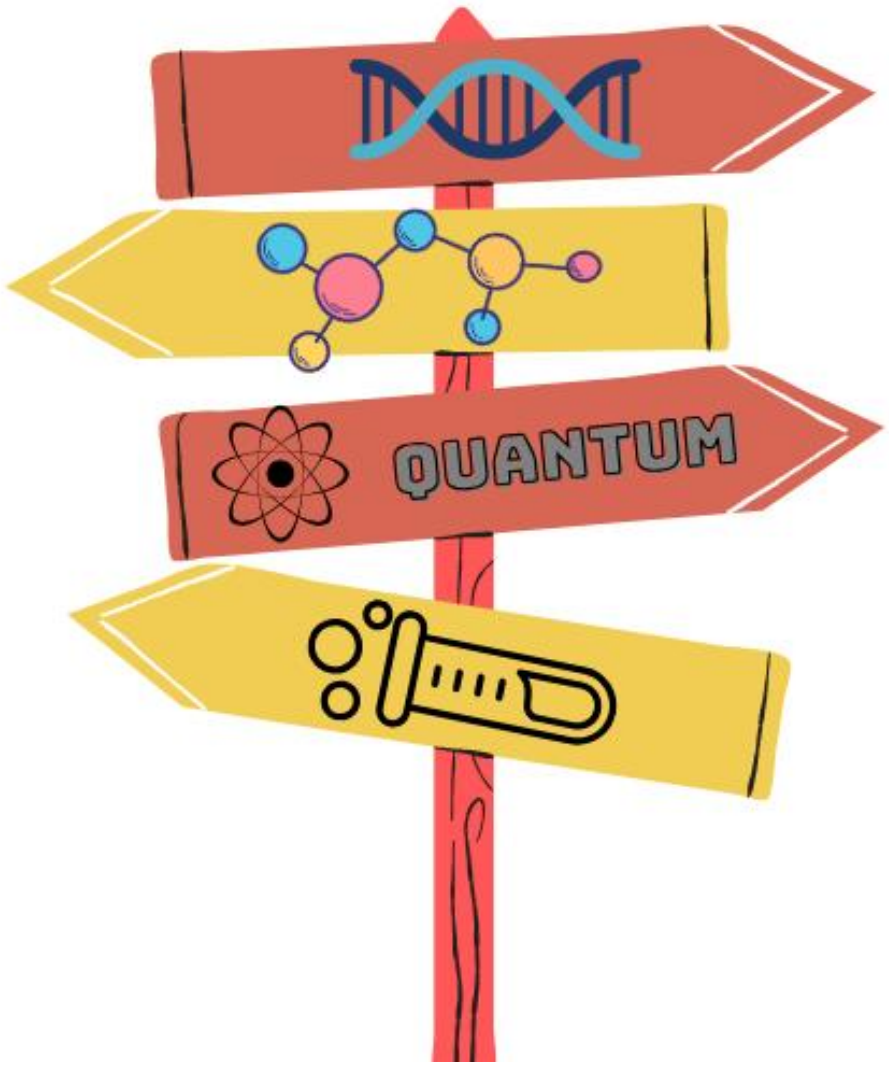
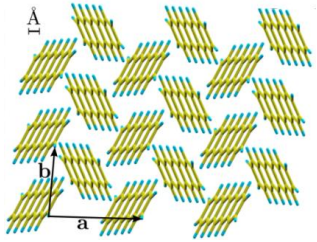


ORIENTATESI

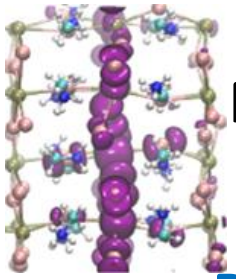
Cdl in Chimica e Scienze Chimiche

Scegli i tuoi esperimenti con...

Francesco Ambrosio



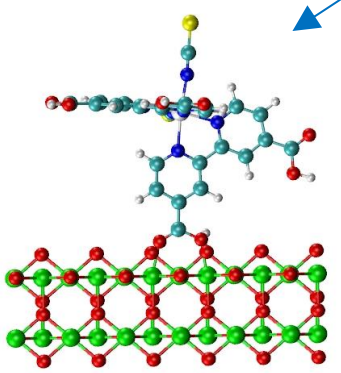
Organic crystals



Metal halide perovskites

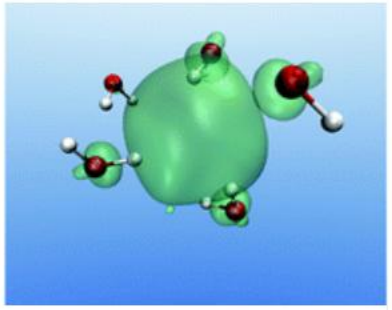
PHOTOVOLTAICS

Dye-sensitized solar cells



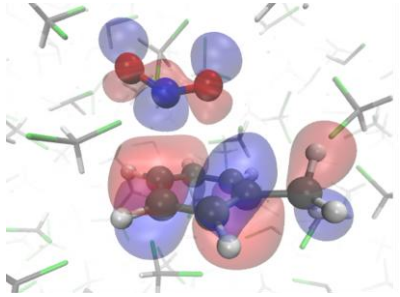
Charge transfer

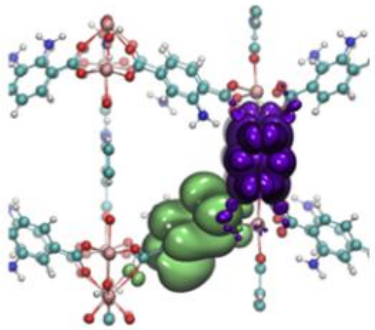
REACTIVITY IN SOLUTION



Hydrated electron

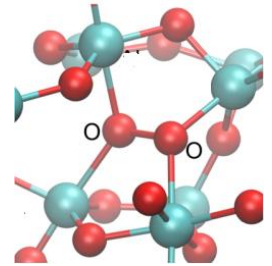
Aromatic nitration



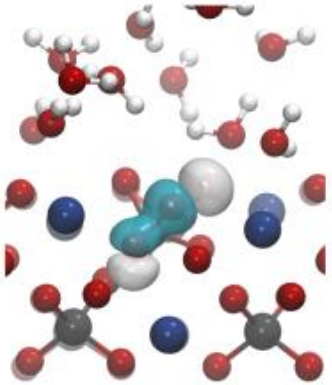


Metal-organic frameworks

Barrier-type amorphous oxides

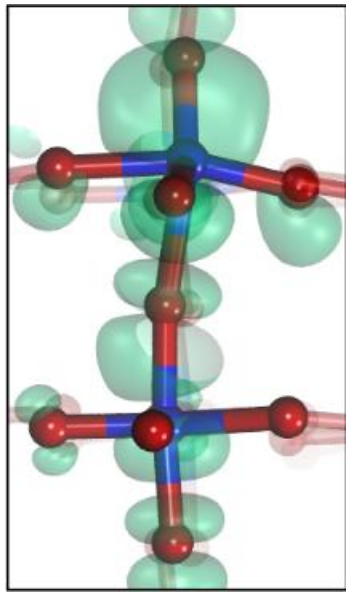


PHOTOCATALYSIS



Semiconductor-water interfaces

Methods

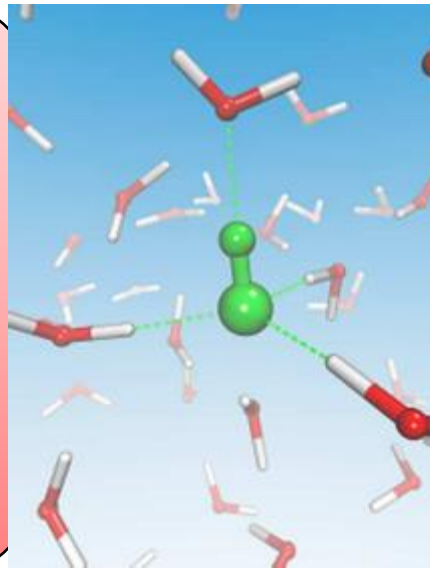


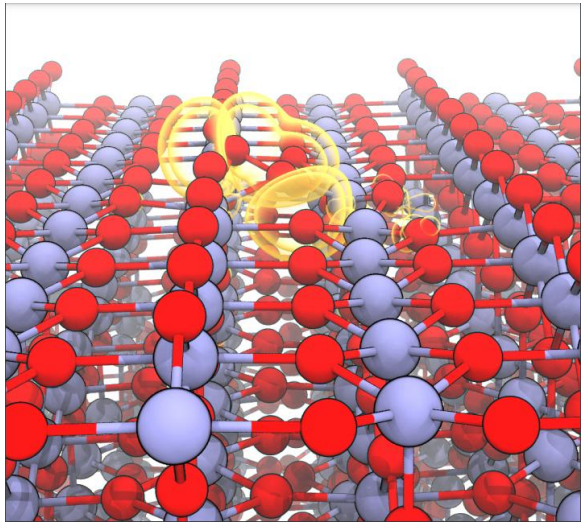
Electronic-structure calculations

- Density functional theory (DFT)
- Time-dependent DFT
- GW approximation
- Post Hartree-Fock methods

Molecular dynamics simulations

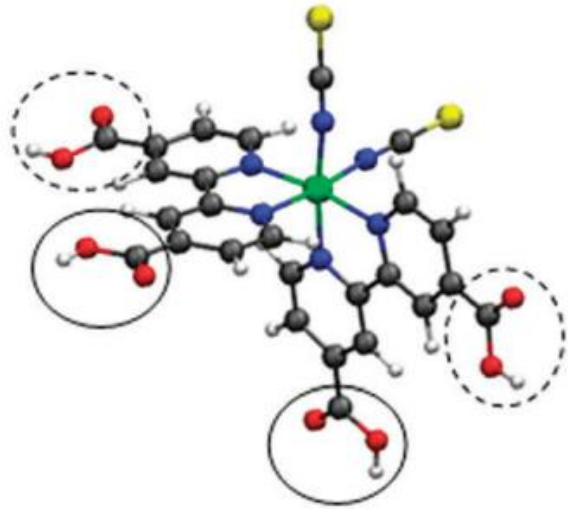
- Thermodynamic integration
- Blue Moon simulations
- QM/MM dynamics



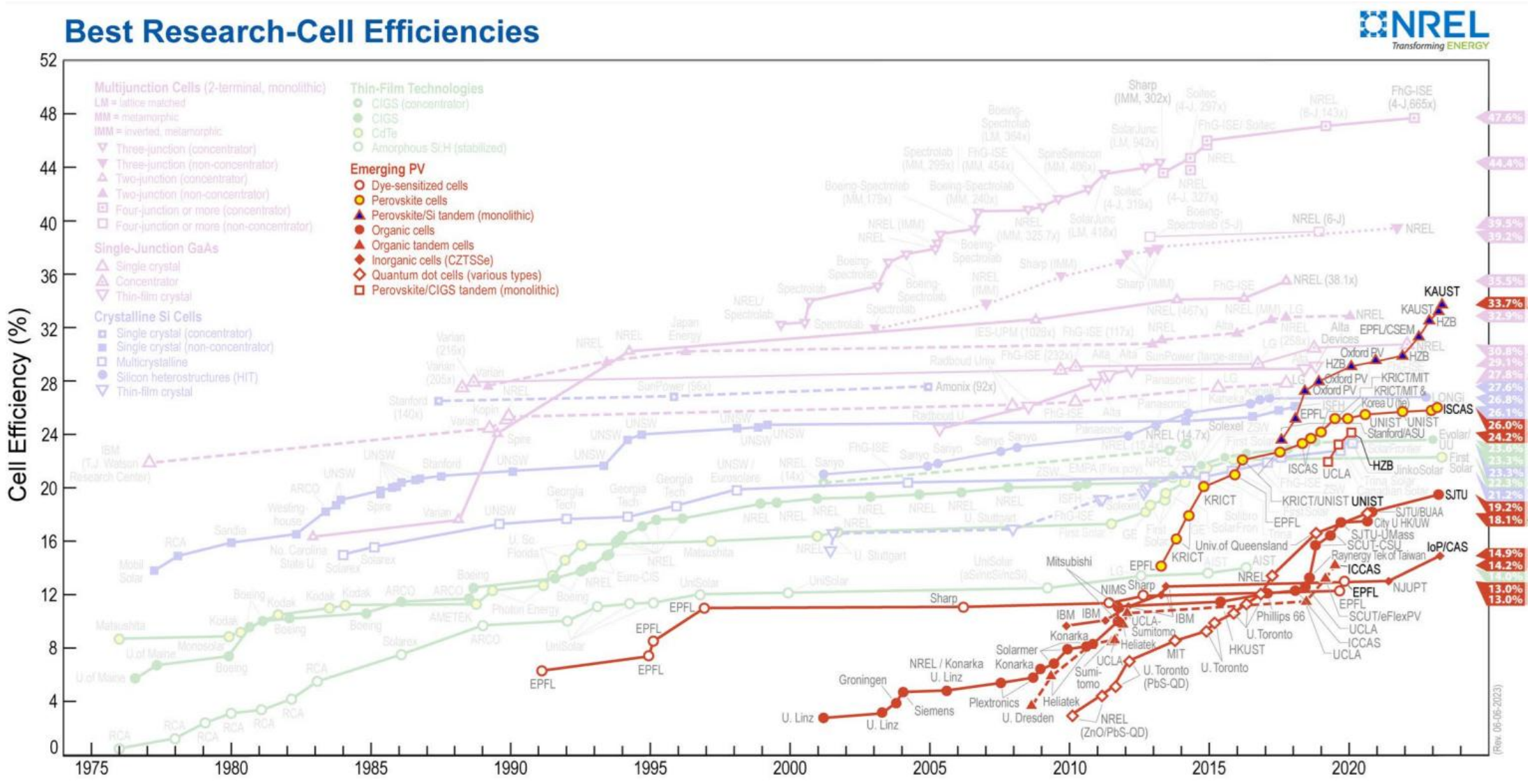


Theoretical modeling

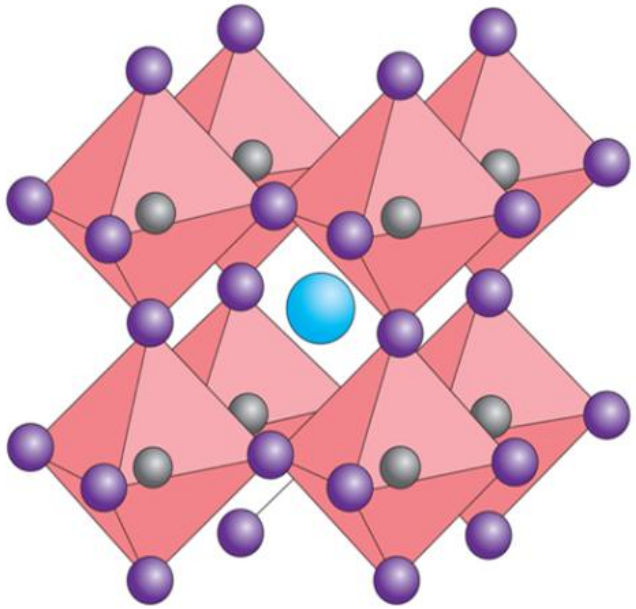
- Electron transfer theory
- Theory of defects in solids
- Model Hamiltonians



Third-generation photovoltaics



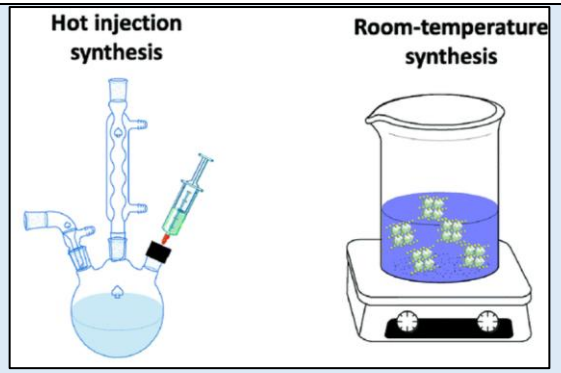
Metal halide perovskites



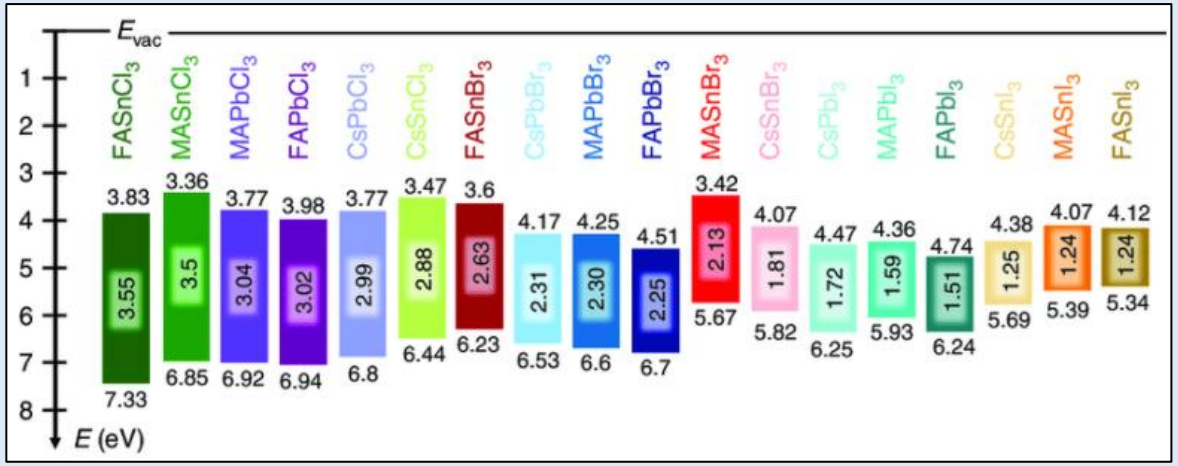
A-site cation
(Cs, $CH_3NH_3^+$…)

X Alogen (I, Cl, Br)
B Metal (Pb,Sn)

- Easily synthesized

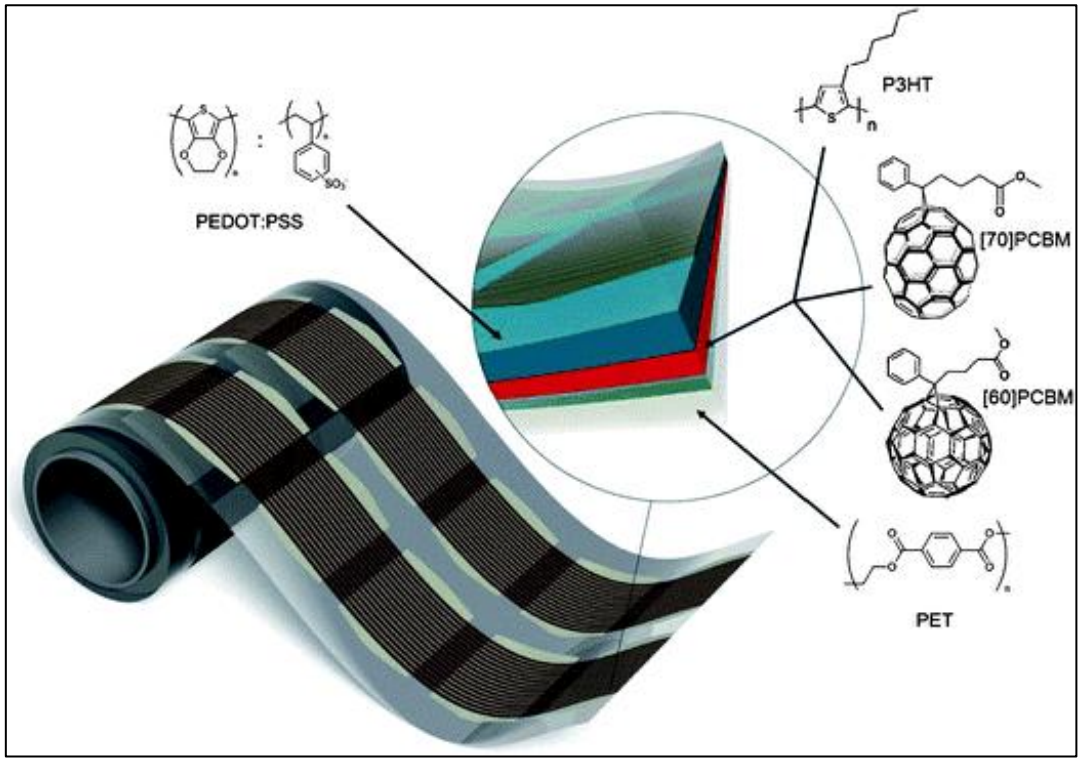


- Highly tunable electronic properties

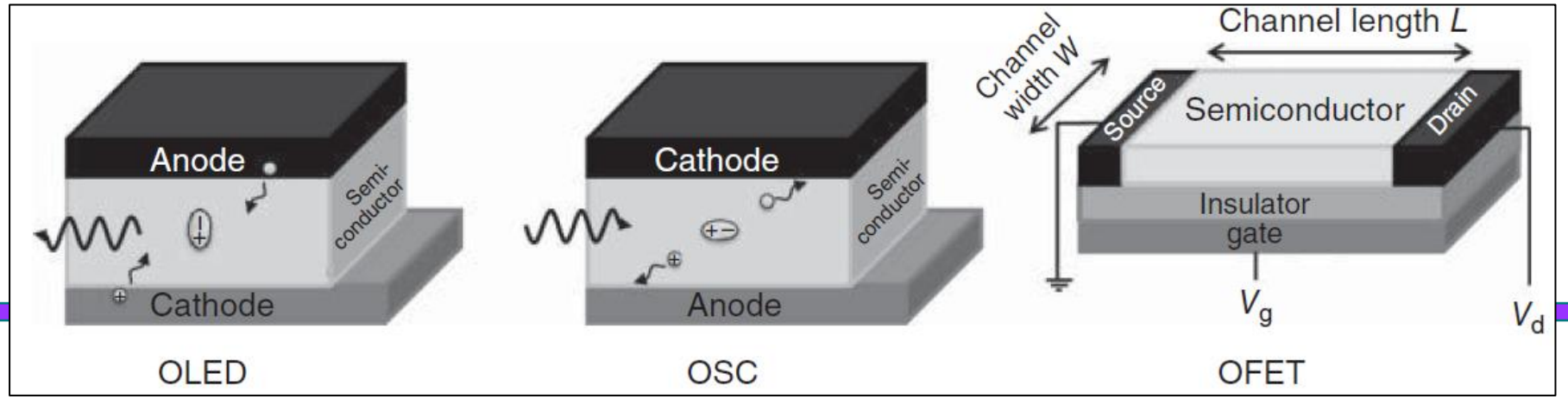


- Numerous possible applications

Organic semiconductors

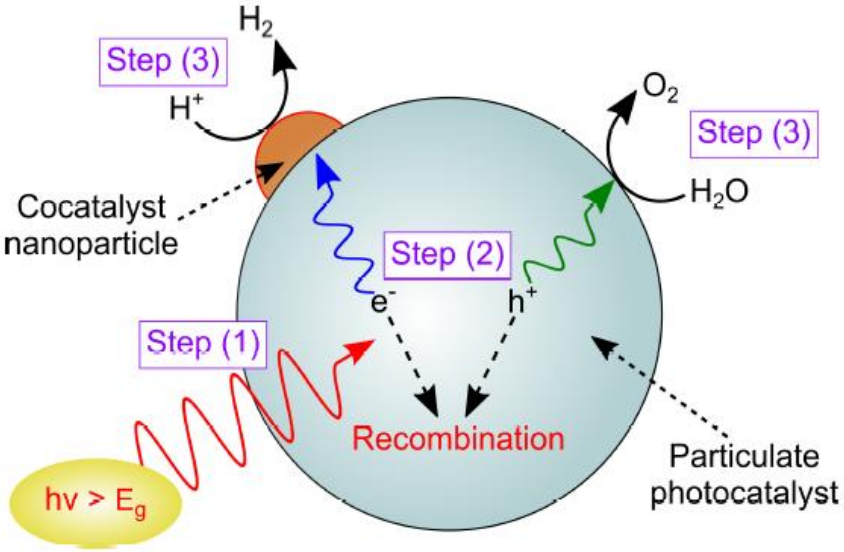


- Processed at low temperatures
- Deposited on high-dimension plastic substrates
- Tunable chemico-physical properties
- Flexibility!



Artificial photocatalysis

Principle: Breaking/forming chemical bonds by solar energy conversion as done by nature



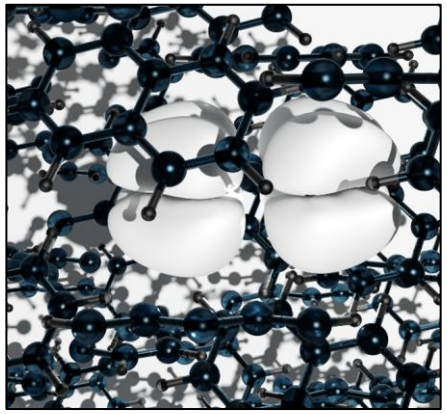
Goals

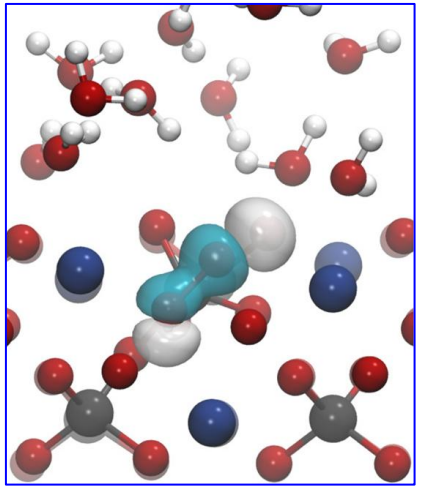
- H_2 from H_2O splitting
- NH_3 from N_2 fixation
- Clean production of fuel/chemicals
- Degradation of pollutants
- CO_2 reduction
- Organic pollutants

Ecological transition!

Available projects

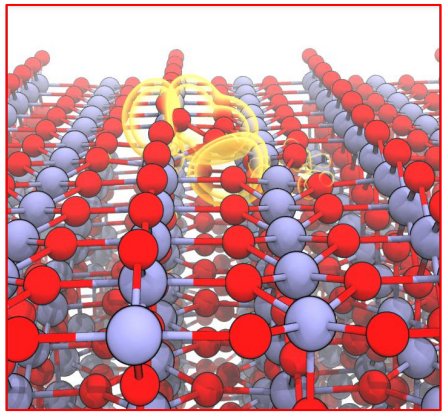
Charge and exciton localization in molecular crystals

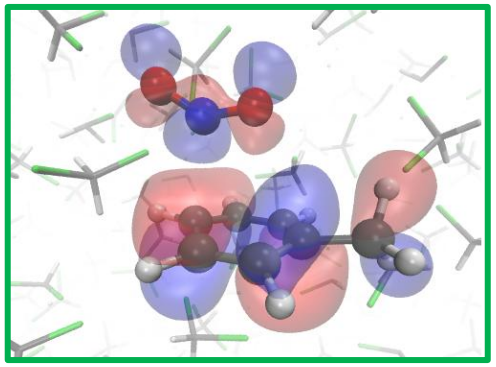




(Photo)catalysis at the liquid-solid interface

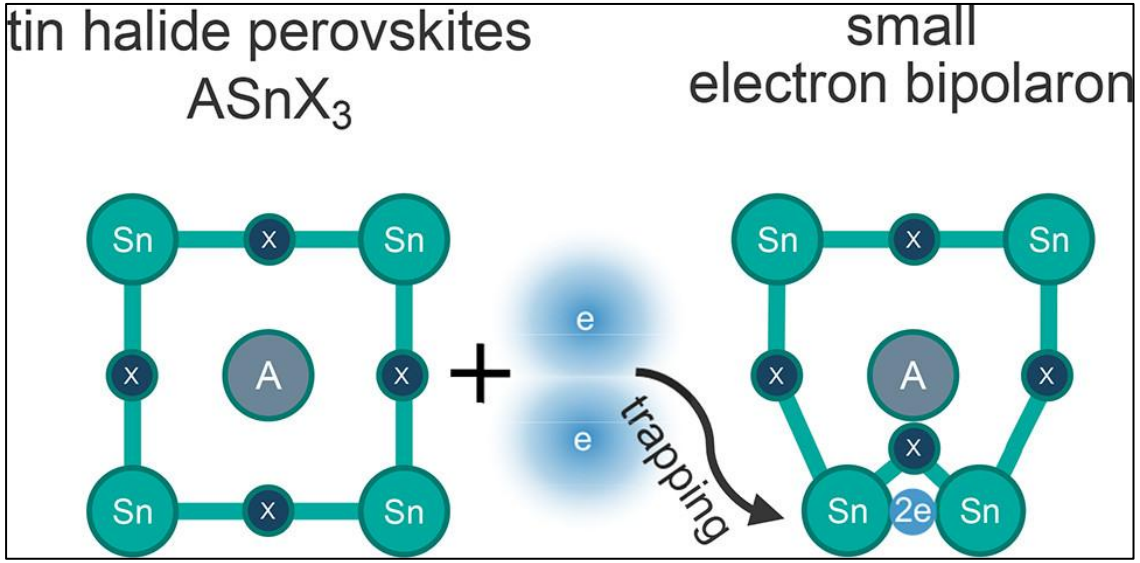
Surface polarons and defects in semiconductors





Redox reactions in solution

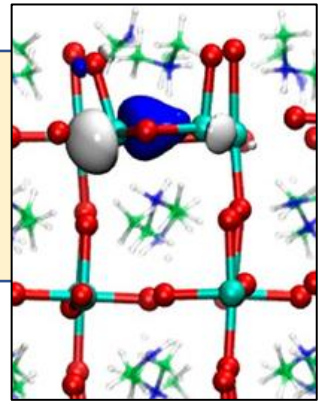
An example of project: bipolarons in perovskites



J. Phys. Chem. Lett. 2021, 12, 22, 5339–5343

	E_b (eV)
$CsSnI_3$	−0.35
$CsSnBr_3$	−0.80
$CsSnCl_3$	−1.43
$CsSnBr_3$	−0.80
$MASnBr_3$	−0.46
$FASnBr_3$	− 0.68
$DMASnBr_3$	−0.51

Idea: Electrons can be trapped at the surface as small bipolarons.

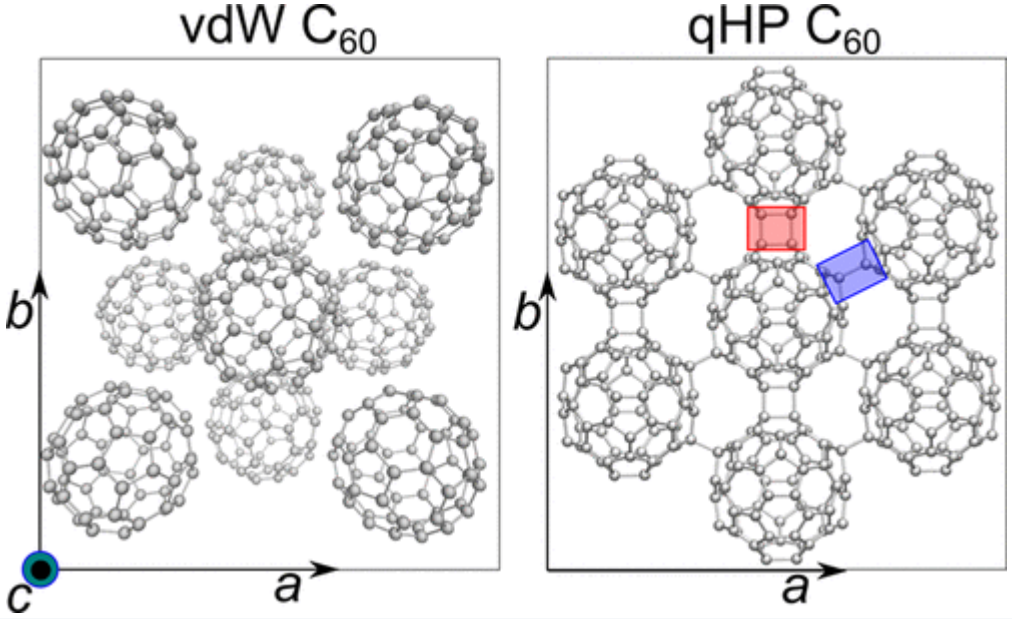


Bipolarons are recurrent in THPs!

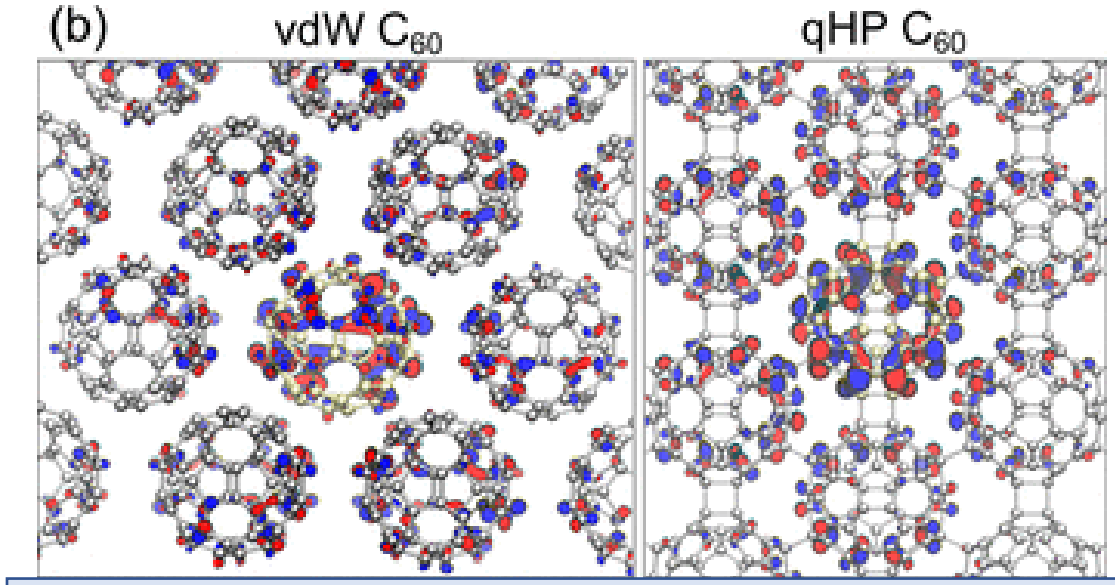
Hotspots for reaction

ACS Energy Lett. 2022, 7, 4, 1308–1315

Another example of project: charge localization in graphullerene



From fullerene to 2D graphullerene…what about the electronic properties?



Similar polaronic charge localization but…

	path	*J*	*k*	*D*	μ
vdW		0.033	1.3×10^{13}	2.15×10^{-6}	0.84 (0.08−0.3)
qHP	c	0.081	9.28×10^{13}	1.85×10^{-5}	7.20 (5)
	s	0.075	8.15×10^{13}		

…different charge mobilities!

Thank you for your attention

Funding

erc

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