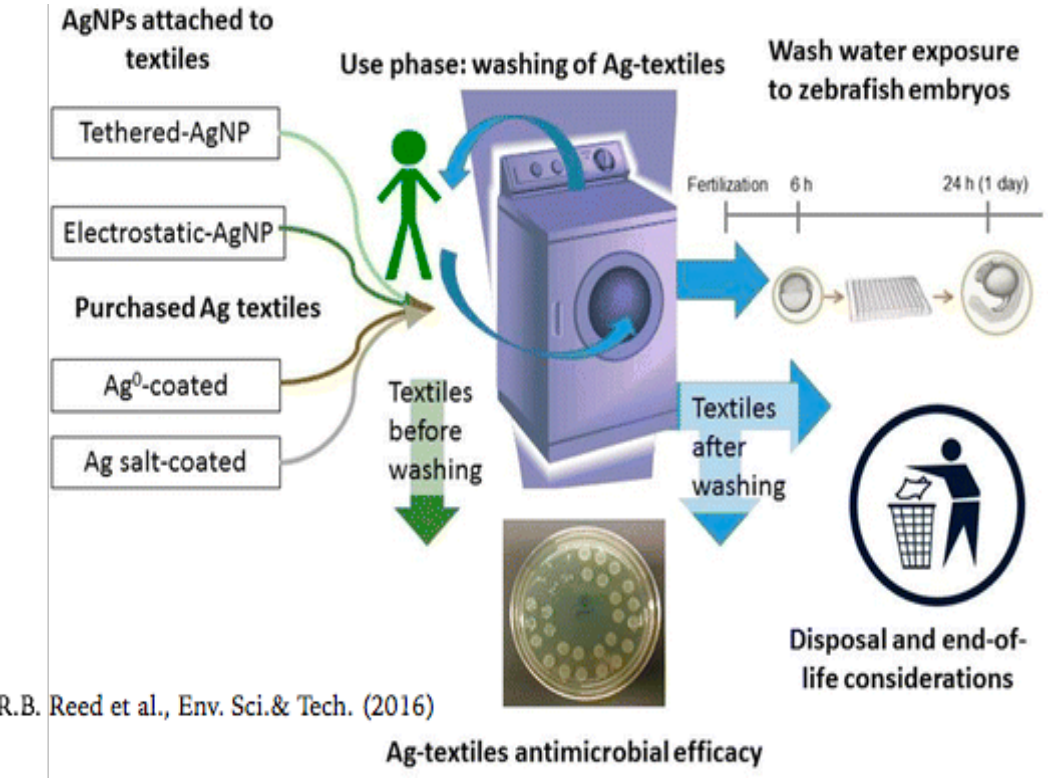
Modelling ‘Magic’ nanoparticles

Using versatile classical molecular dynamics software to study structural stabilities and instabilities at the nanoscale. Interfacing them with ab-initio codes, it then unravels how the intrinsic morphological diversity can be exploited to tune chemical physical properties of nanoparticles

The good, the beautiful and the bad

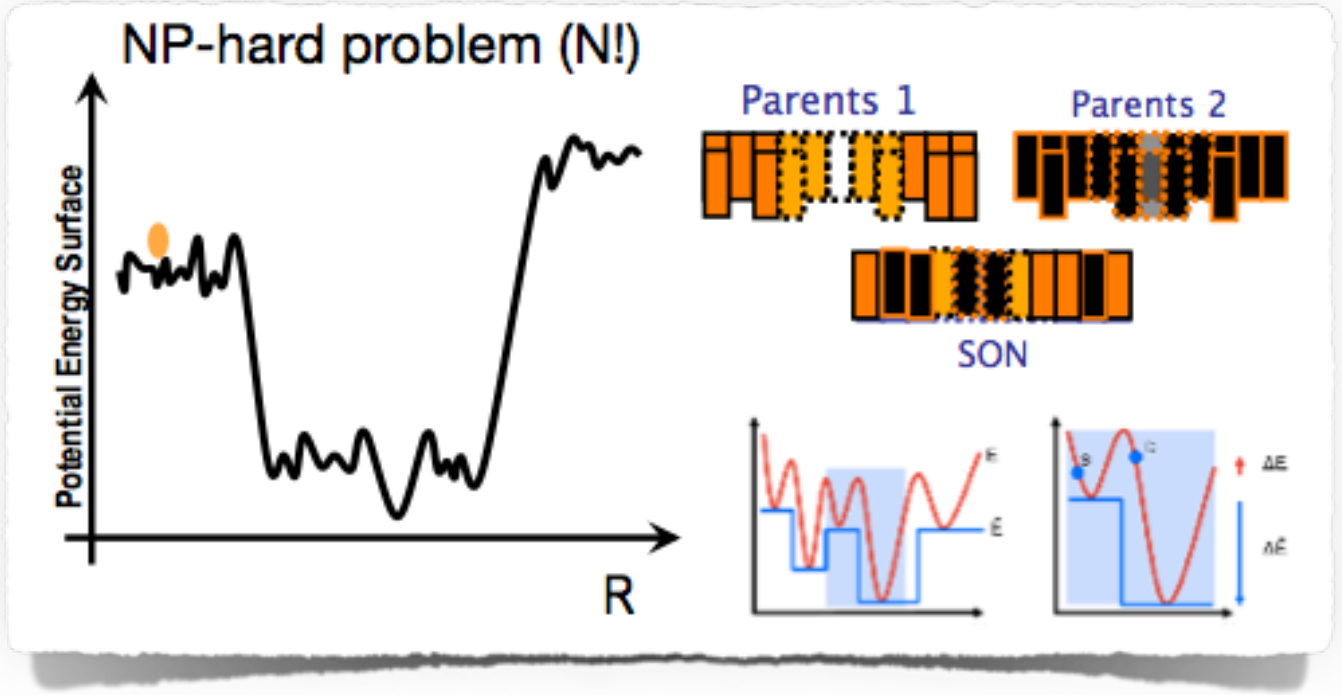


R.B. Reed et al., Env. Sci.& Tech. (2016)

A. Ruditskiy, Y. Xia, ACS Nano (2017)

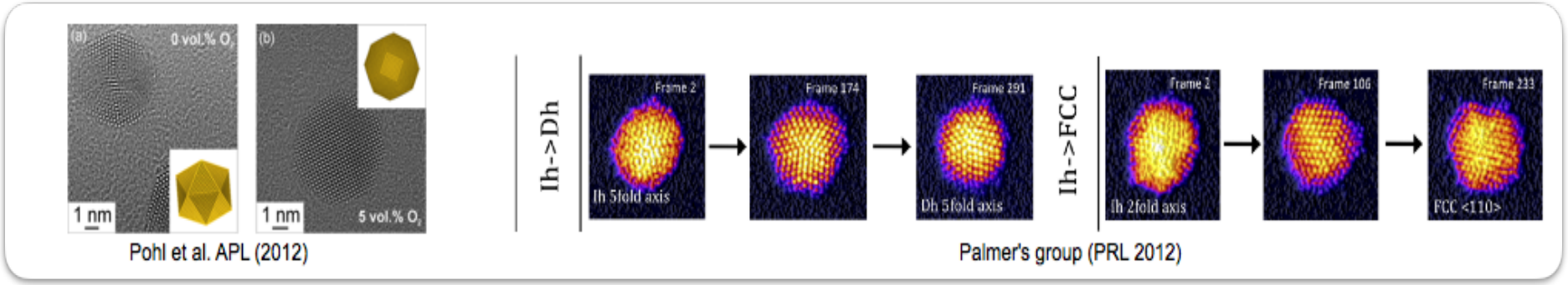
Towards the design of nanocatalysts

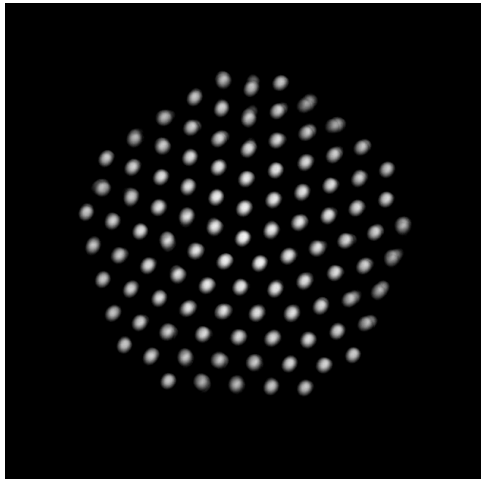
"Before anyone can study a material using software, they first have to construct the material and know the position of the various atoms" by S. B. Bennett (Materials Science News, 1 June 2017)



Wales, Johnston, and Ferrando's groups

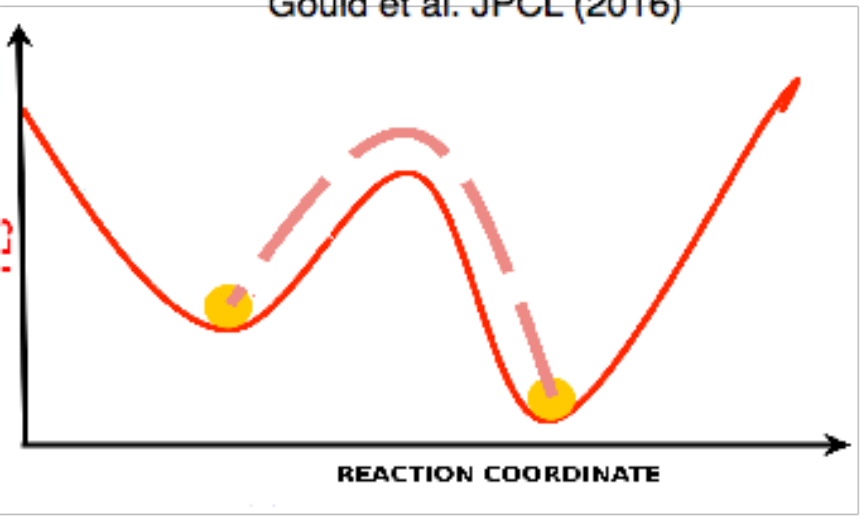
Towards the design of nanocatalysts





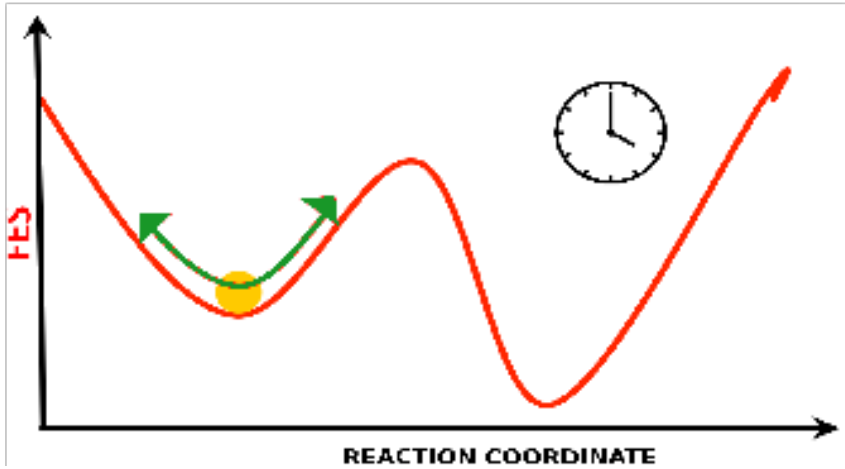
Double-ended transition path-sampling

Gould et al. JPCL (2016)



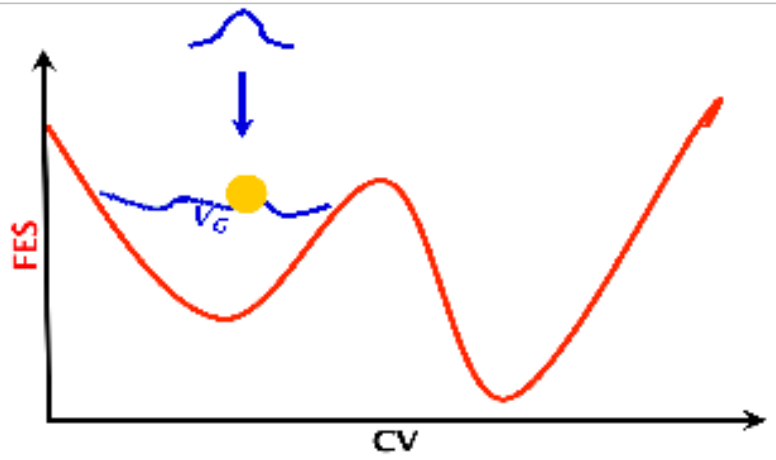
Increasing temperature Molecular Dynamics

Pavan et al, PCCP(2015)
Rossi et al. JPCM (2017)

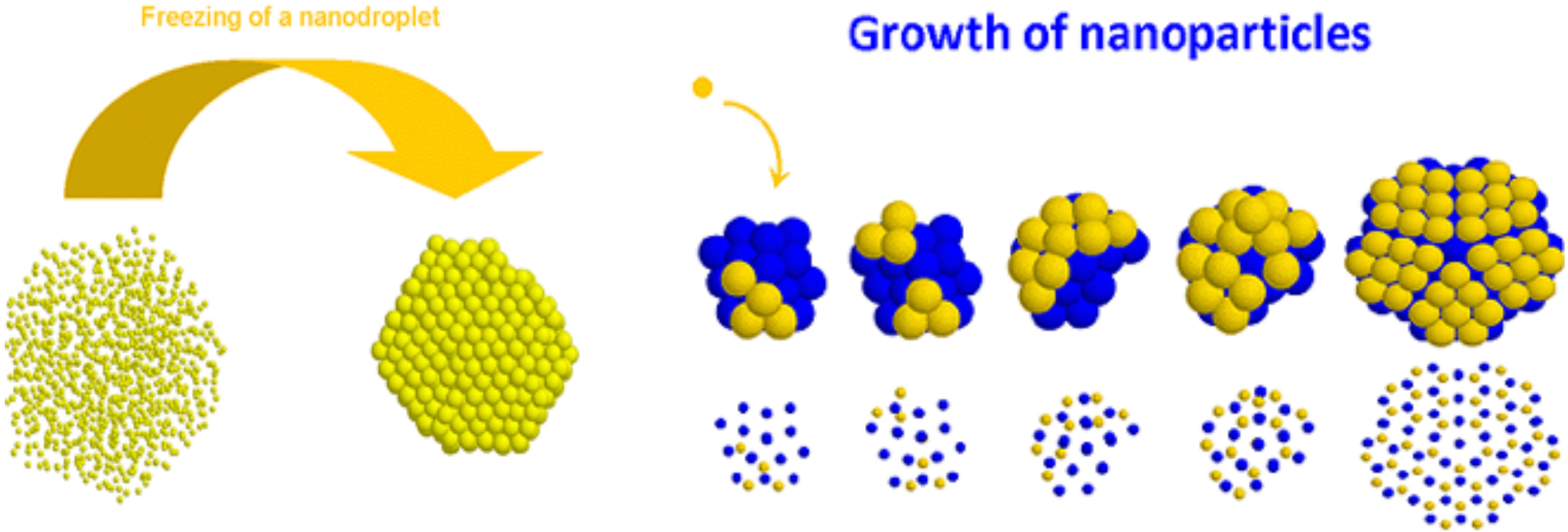


Metadynamics

Pavan et al, JCP(2015)
Rossi et al., PCCP(2017)
Pavan et al. EPJD (2013)



Design and formation process(es)

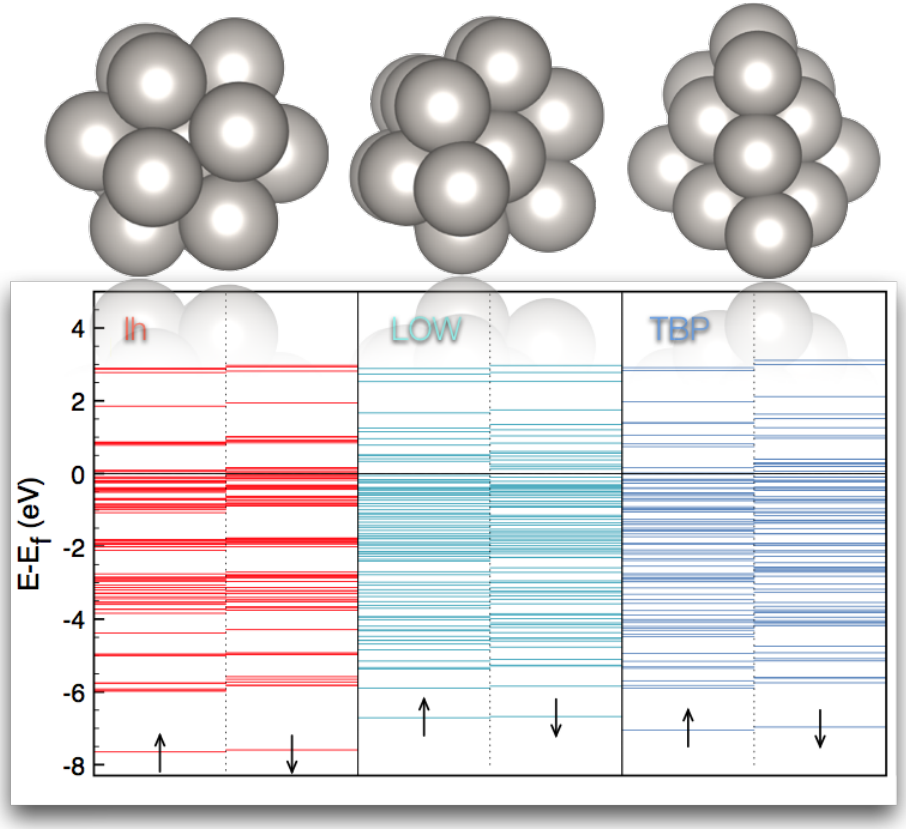


Modelling growth and thermal stability, detecting new structures and chemical orderings

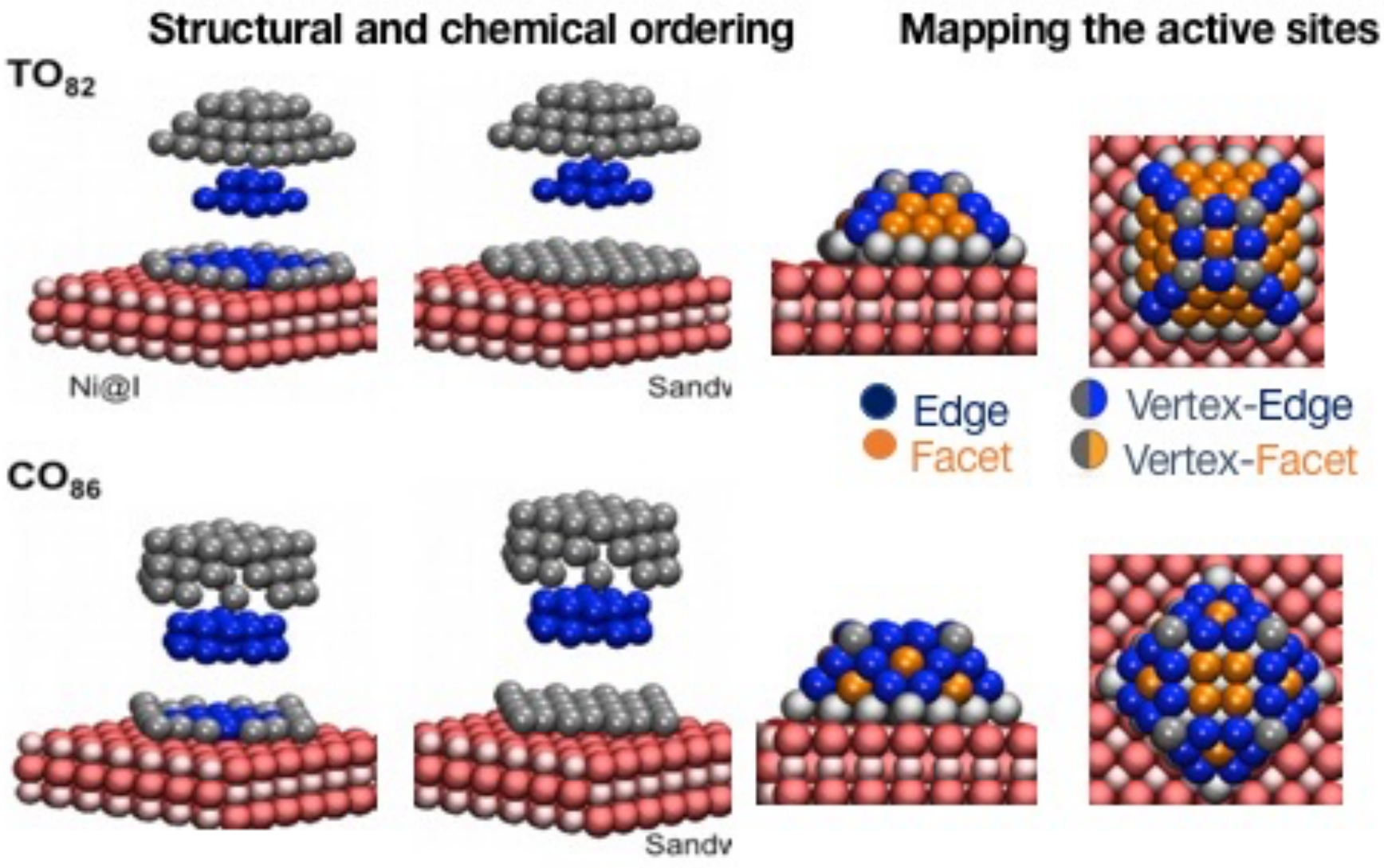
RMP 77 (2005) 371; JCP 116 (2002) 3856; JPCC 114 (2010) 1504; Nanoscale 4 (2012) 1160

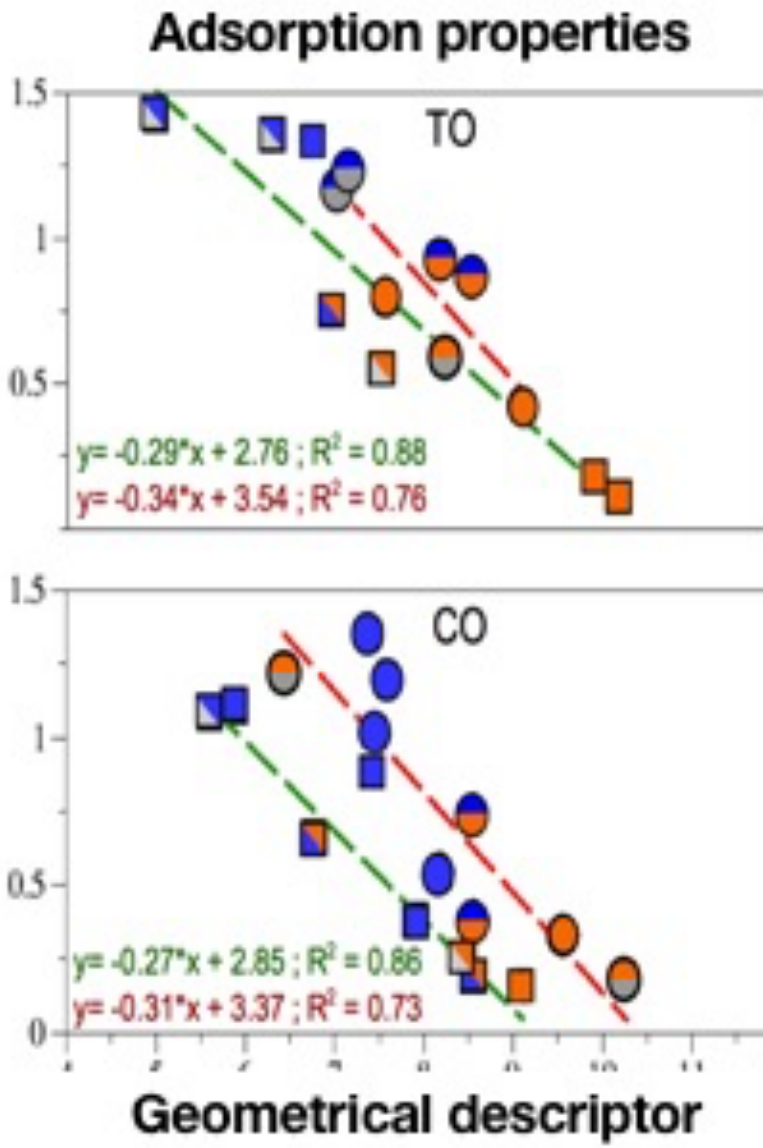
Towards physical properties

$$\hat{\mathcal{H}}\Psi = E\Psi$$



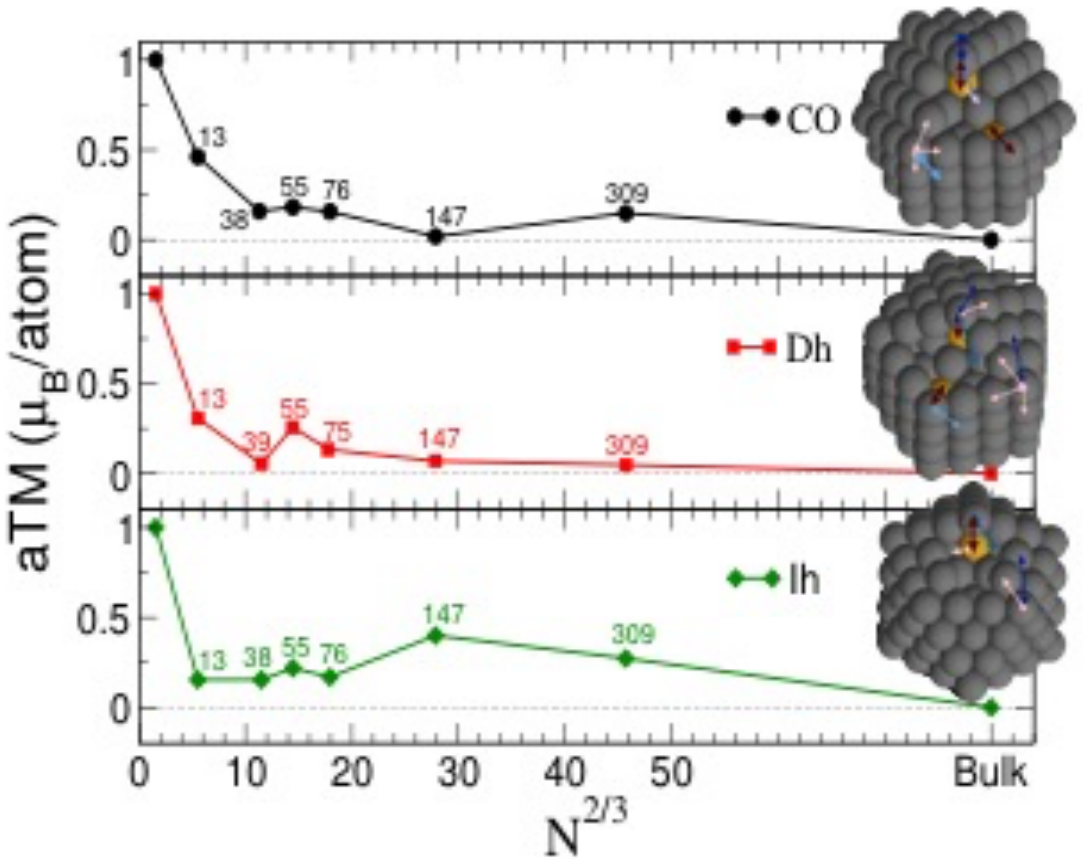
Magic shapes & nanocatalysis

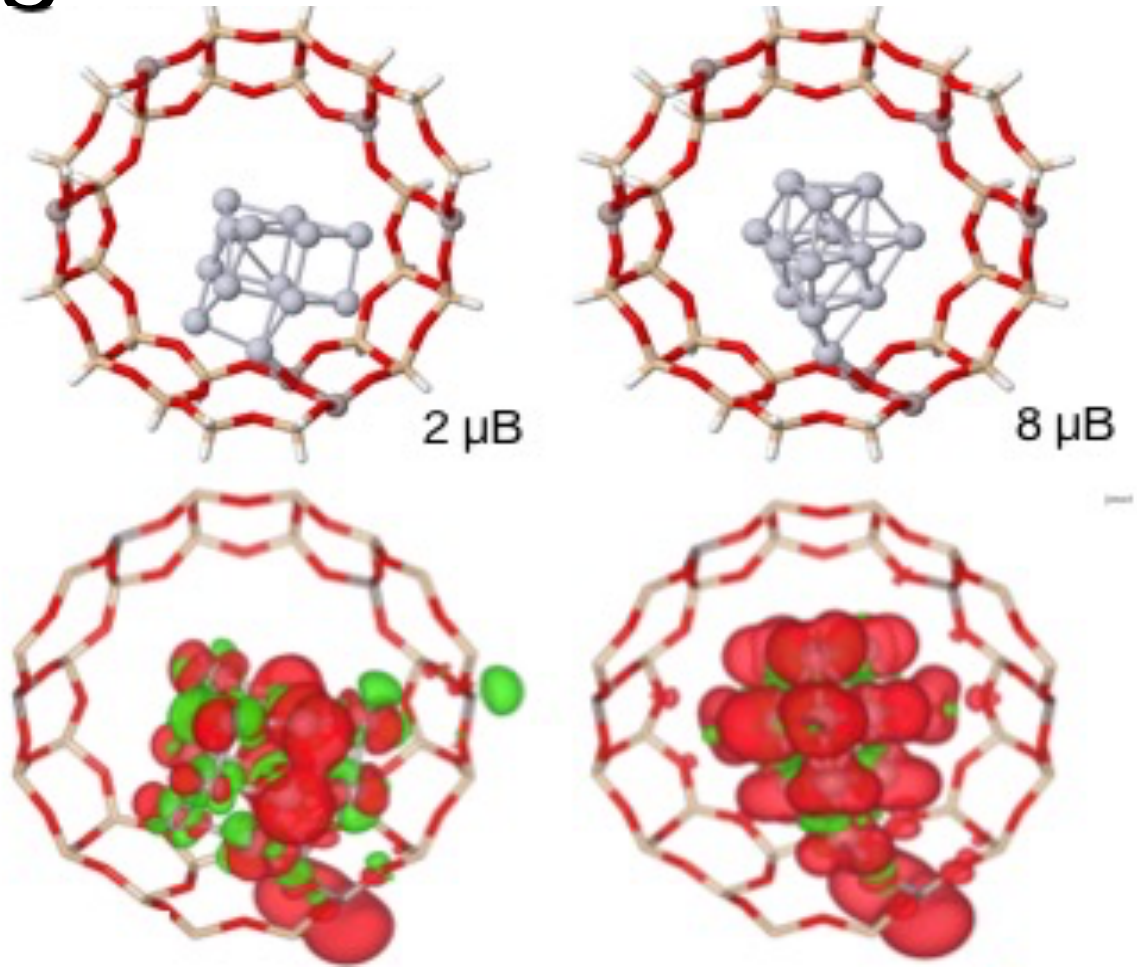




ACS Cat. 6 (2016) 4388, PCCP 13 (2011) 7701, Inorganics (2017)

Magic shapes & nanomagnetism





Nano Letters 16 (2016); EPJD (2013); Nanoscale (2012); Nanoscale under review

Total magnetization and average coordination increase

Present & Future

Numerical modelling tools arising from the combination of classical and ab-initio techniques, which need computational facilities like the MMM-Hub “Thomas”, will guide and help experiments to discover properties of nanoparticles at the atomistic level, and to propose how to tune them for target applications.