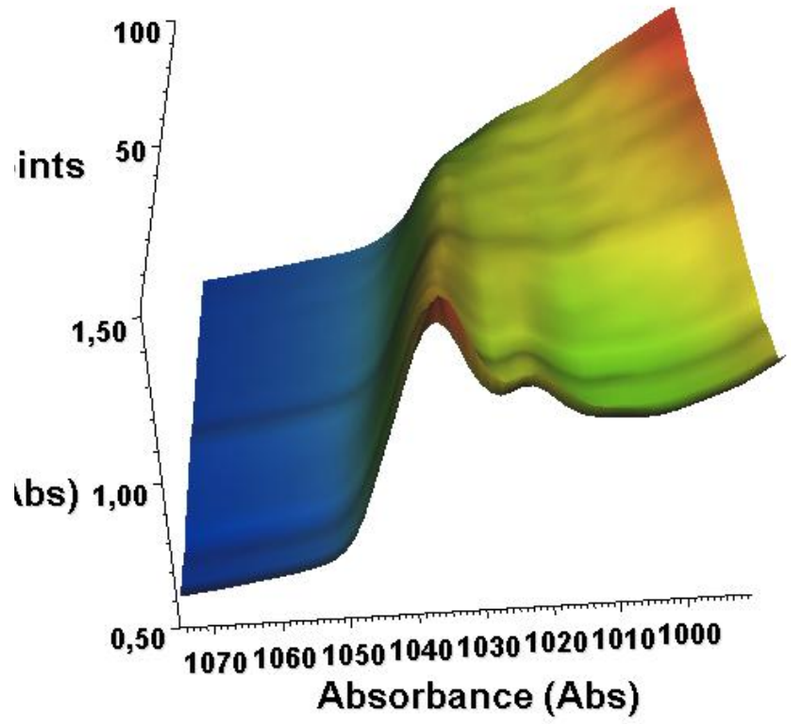
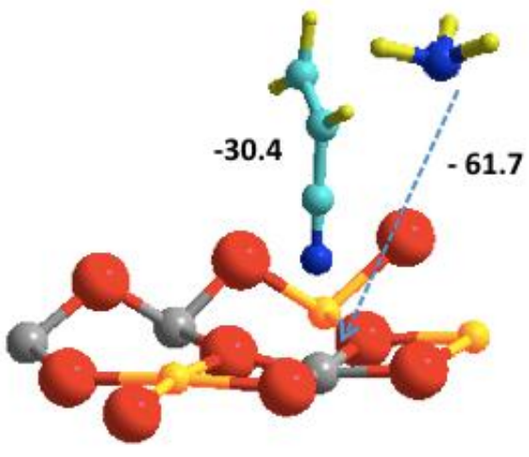
Nano, atomic, molecular and long range *Operando* Characterization DURING Materials Processing

Bridging the gap between *in situ* characterization and computational modelling of functional nanomaterials during processing





Miguel A. Bañares

CSIC-Institute for Catalysis, Madrid

Materials Ontology Workshop

DG RTD, CDMA-SDR-1, Brussels

29.6.2018

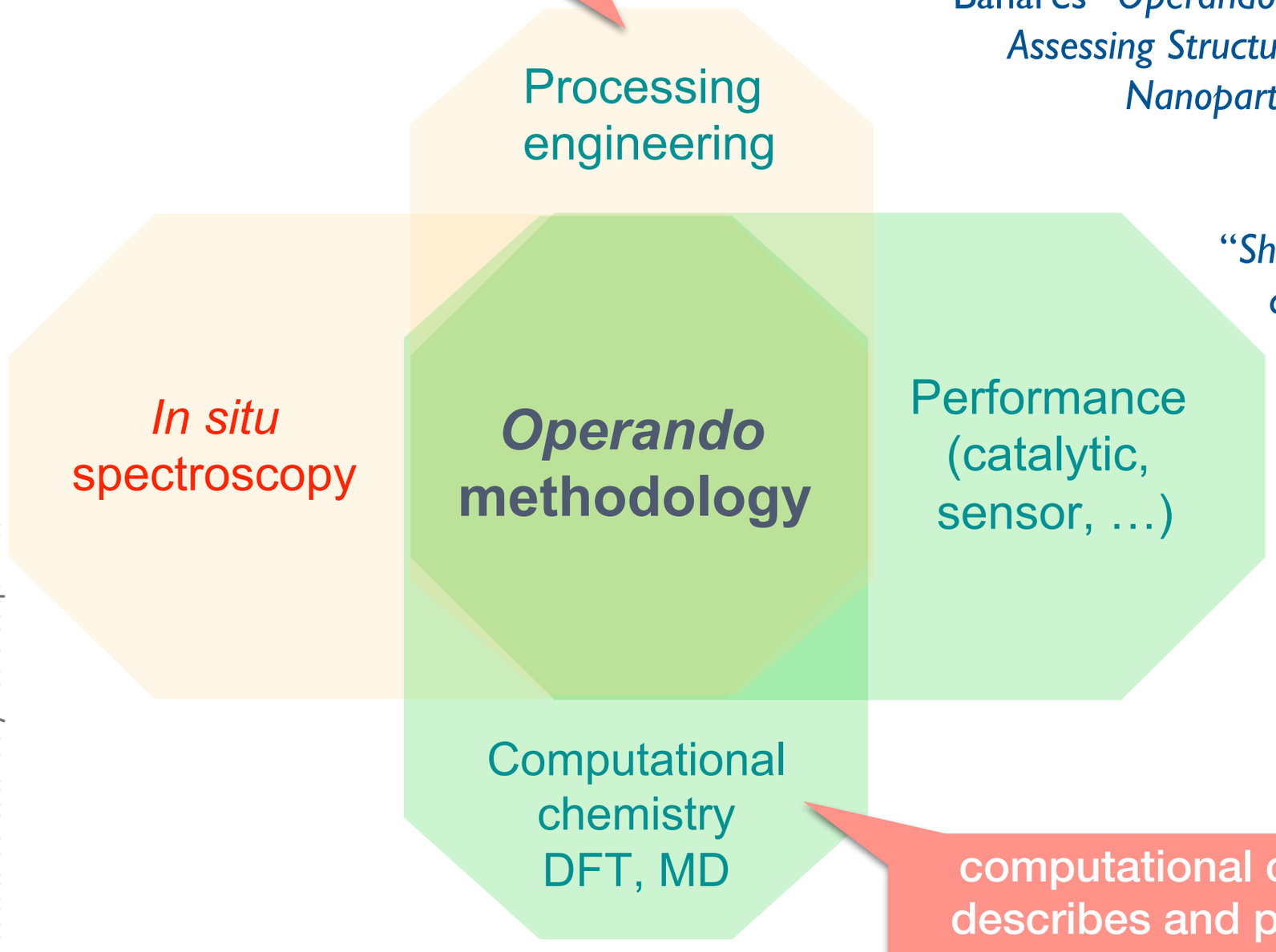
Miguel A. Bañares
Instituto de Catálisis y Petroleoquímica

CSIC
Consejo Superior de Investigaciones Científicas

Catalytic Spectroscopy Laboratory

Operando methodology: determining structure (atomic, molecular, nano) and performance during actual working (*operando*) conditions

Reproducing genuine materials processing conditions



computational chemistry brings rationale, describes and predict structures, spectra, reactivities

Bañares and Daturi, *"Understanding catalysts by time-/space-resolved operando methodologies"*, ***Chem.Soc.Rev. (2018)***, invited review, submitted

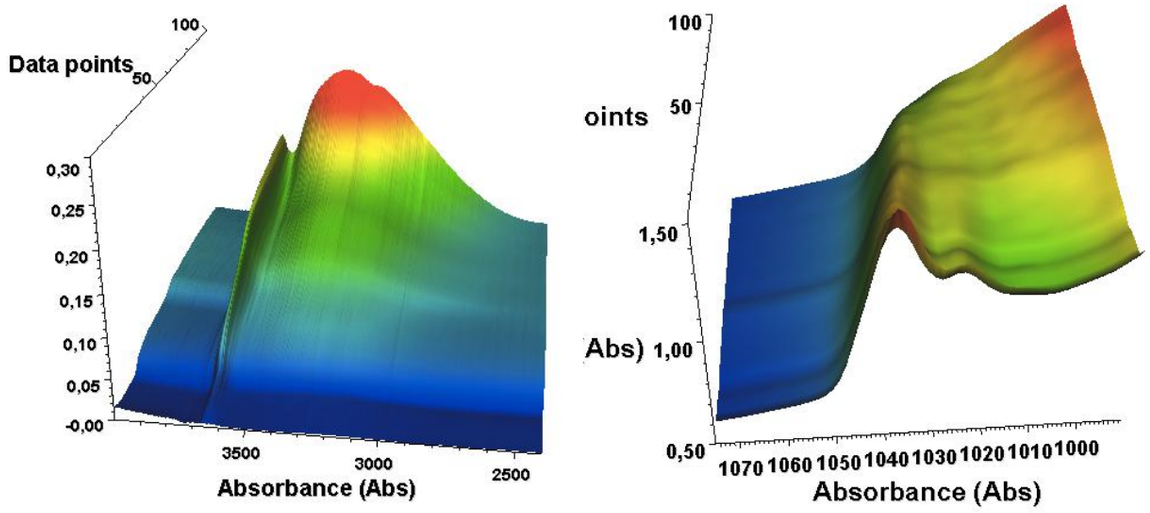
Bañares "*Operando* Spectroscopy: *the Knowledge Bridge to Assessing Structure–Performance Relationships in Catalyst Nanoparticles*", **Adv. Mater.** 23 (**2011**) 5293

Bañares, Rasmussen, Daturi et al. "*Shaping up operando spectroscopy: Raman characterization of a working honeycomb monolith*". **Catal. Sci. Technol** 5 (**2015**) 4942-4945
LARGE SCALE SHAPED MATERIAL

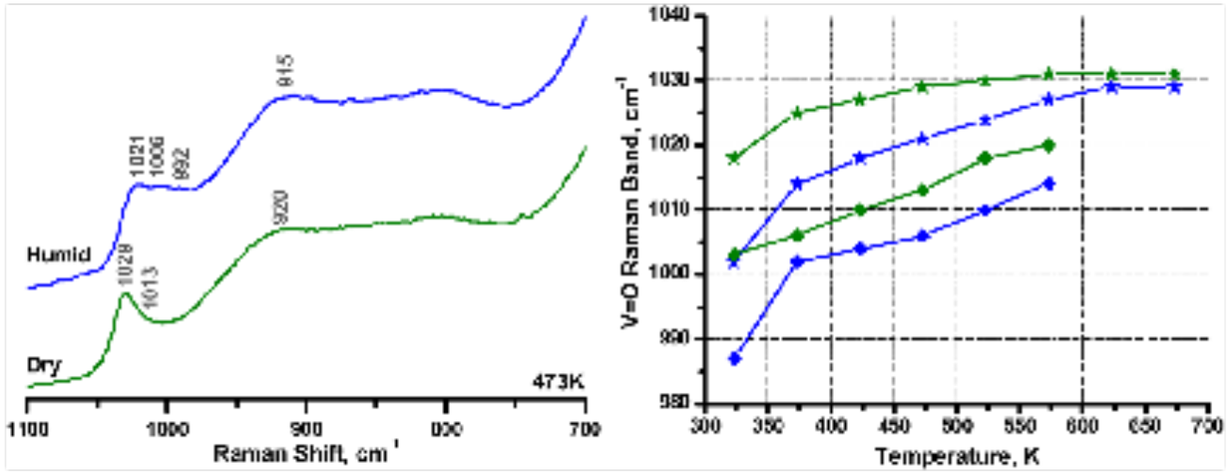
Bañares, Wachs et al. (**2017**) "*A decade+ of operando spectroscopy studies*". **Catalysis Today**, 283, 27

Miguel A. Bañares
Instituto de Catálisis y Petroleoquímica
CSIC
Consejo Superior de Investigaciones Científicas

In situ Raman and in situ infrared backed up by DFT-Molecular Dynamics description of hydroxylation-hydration of molecuarly dispersed vanadium oxide on titania surface

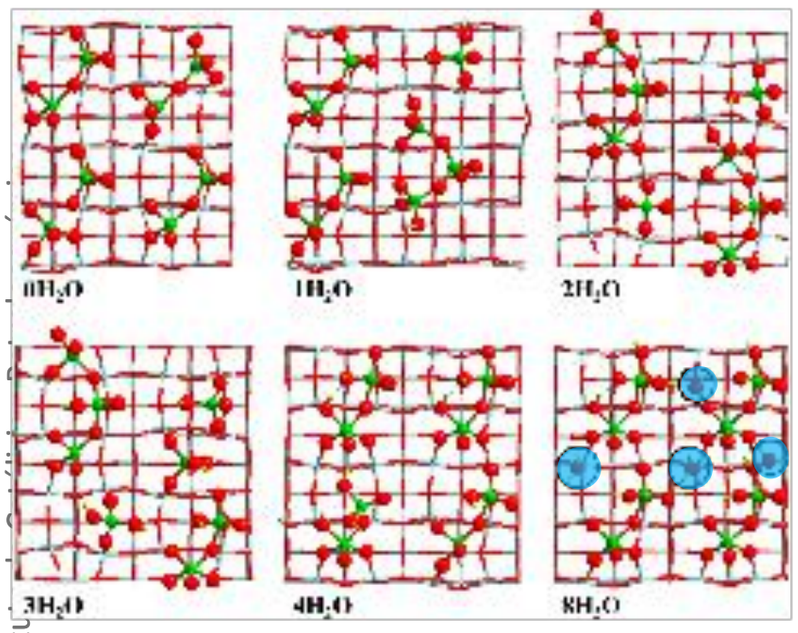


In situ infrared during hydroxylation/hydration

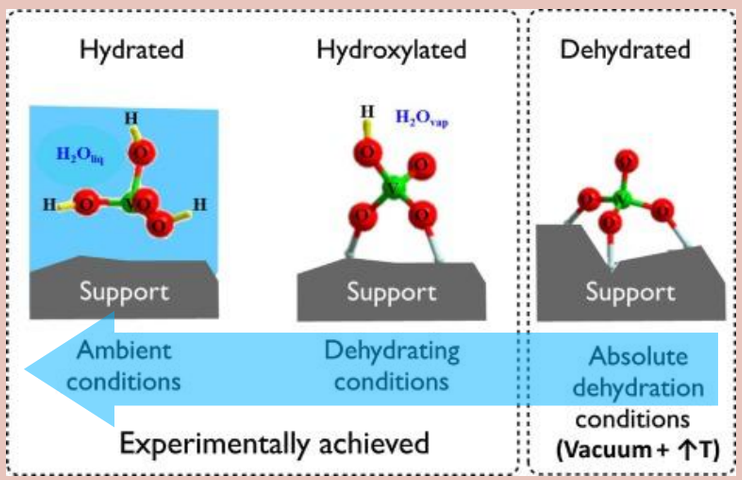


In situ Raman during hydroxylation/hydration

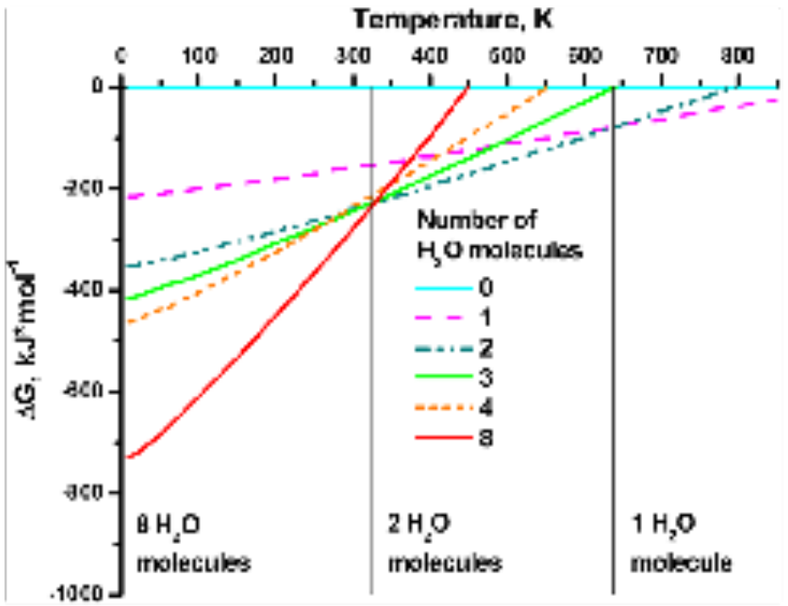
Density Functional Theory



Atomic/molecular scale understanding



Molecular Dynamics



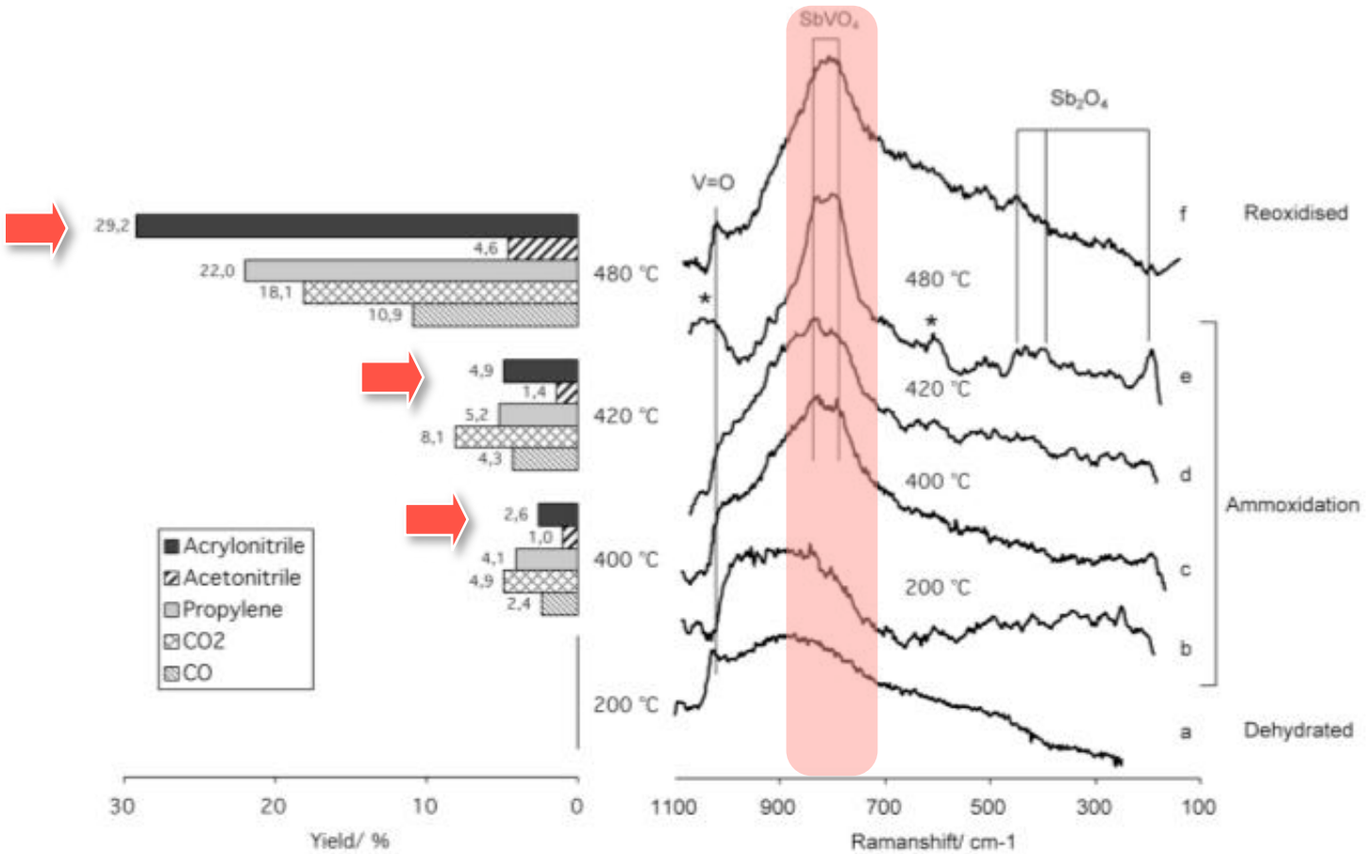
Miguel A. Bañares
Institu
CSIC
Consejo Superior de Investigaciones Científicas

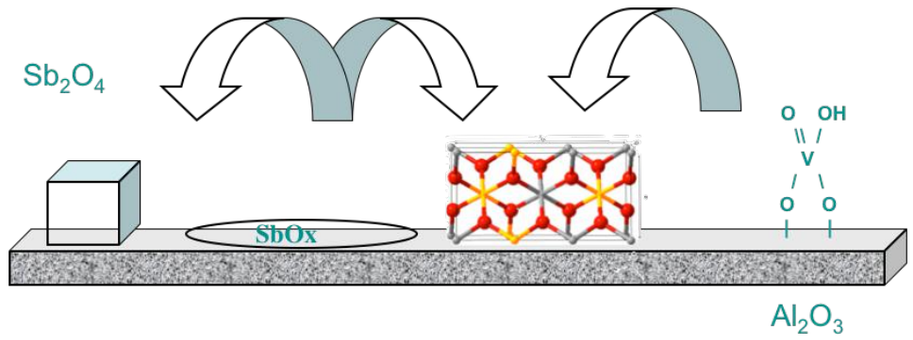
Lewandowska, Calatayud, Tielens, Bañares, M. A. (**2013**). Hydration Dynamics for Vanadia/Titania Catalysts at High Loading: A Combined Theoretical and Experimental Study. **J. Phys. Chem. C**, 117(48), 25535–25544. doi:10.1021/jp408836d

Lewandowska, Calatayud, Tielens, Bañares, **J. Phys. Chem. C** 2011, 115 (**2011**) 24133–24142

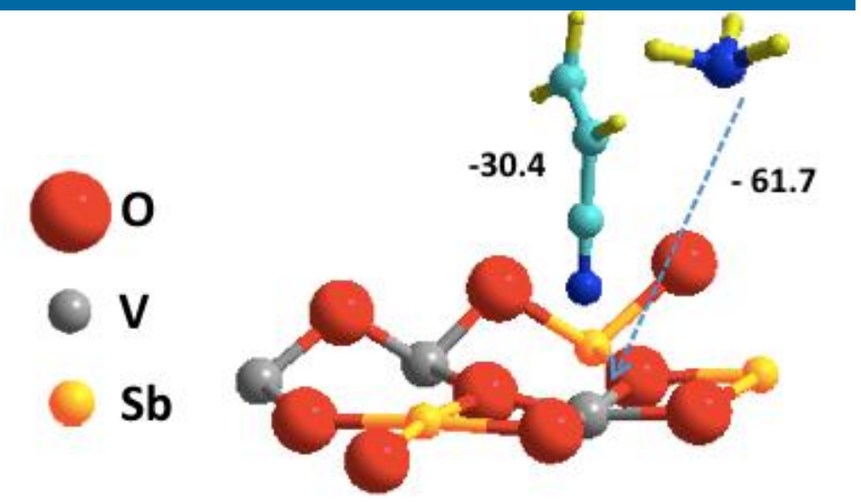
Catalytic Spectroscopy Laboratory

Operando Raman-GC and DFT demonstrate that the nature of the active site, the role of dispersed oxides and the role of defects for propane ammoxidation on VSbO4 **nanocyrstals** and **atomically** dispersed VOx on alumina (first *operando* paper)





Atomically dispersed vanadia blends with Sb_2O_4 during g reaction into $VSbO_4$ nanorystals (2002)



Computation DFT show the nature of reactive sites and the role of defects in crystal lattice on reactivity (2012)

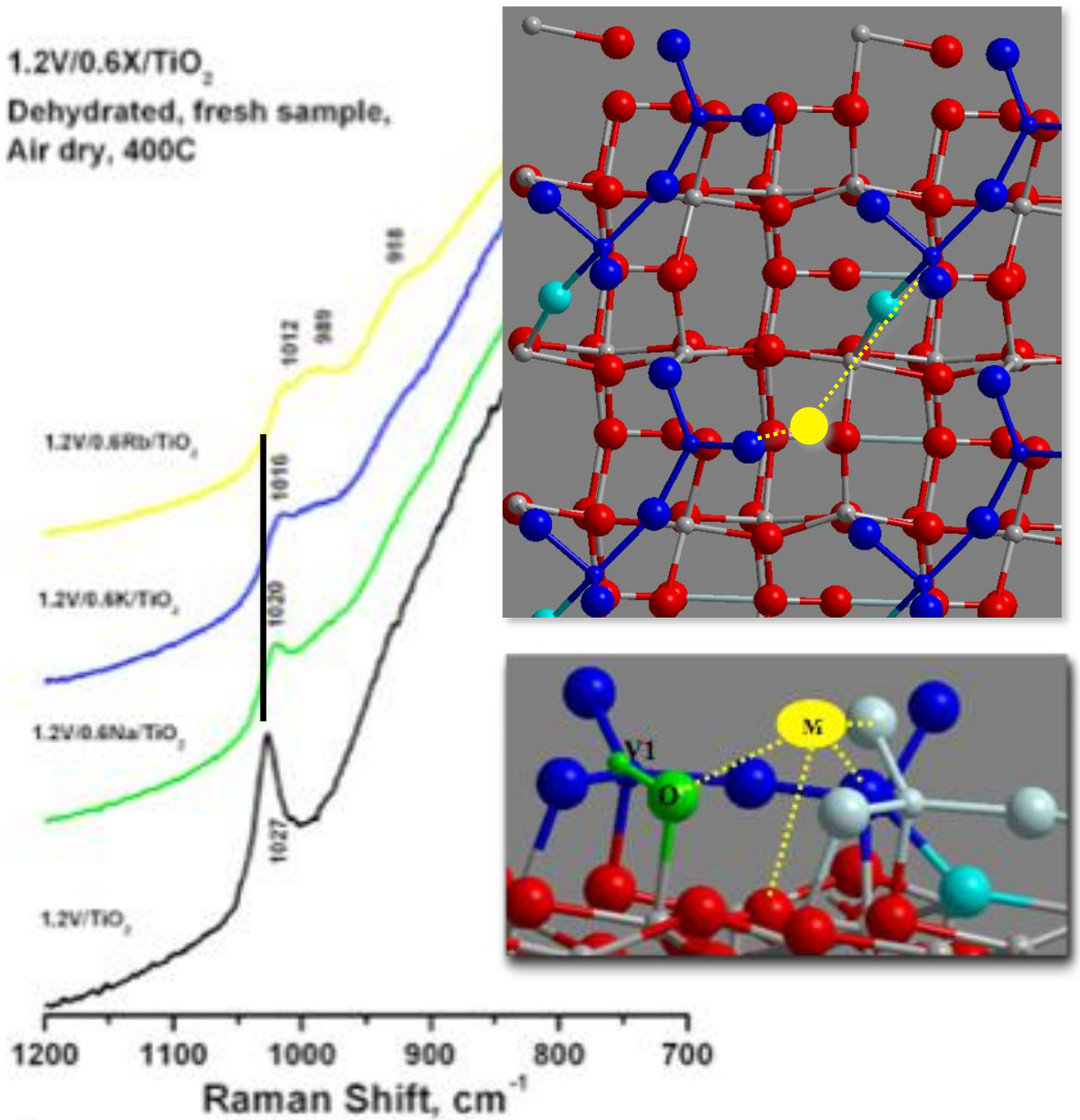
Materials are like people: defects make them interesting

Miguel A. Bañares
Instituto de Catálisis y Petroleoquímica
CSIC
Consejo Superior de Investigaciones Científicas

(**2002**) Guerrero-Pérez, Bañares,"*OperandoRaman study of alumina-supported Sb–V–O catalyst during propane ammoxidation to acrylonitrile with on-line activity measurement*". **Chem. Comm.**, 1292–1293.

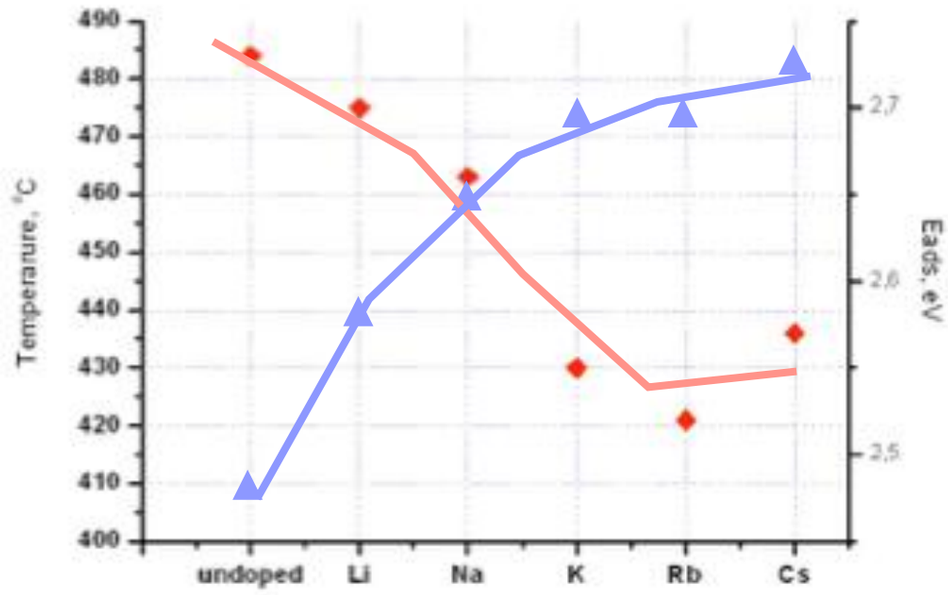
(**2012**) Rojas, Calatayud, Bañares,"*Theoretical and Experimental Study of Light Hydrocarbon Ammoxidation and Oxidative Dehydrogenation on (110)-VSbO 4 Surfaces*". J. Phys. Chem. C, 116(16), 9132–9141. http://doi.org/10.1021/jp3017437

Alkali dopants on structure, reducibility and Raman spectra of vanadia-titania catalysts: Combined in situ Raman and computational chemistry DFT modelling



In situ Raman and DFT modelling demonstrate the weakening of V=O bond due to interaction with alkali cations

Temperature programmed reduction confirms the decrease of reducibility predicted by DFT modelling upon alkali doping of molecularly dispersed vanadia on titania



CSIC
Consejo Superior de Investigaciones Científicas

Catalytic Spectroscopy Laboratory