Red Argentina de Nanociencia y Nanotecnologia. Materiales Nanoestructurados y Nanosistemas

- **Nodo II. Superficies y Recubrimientos**
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Lineas de Investigacion

- Estudio y desarrollo de nuevos materiales utilizando haces de particulas energeticas
- Estudio de superficies cristalinas puras y con adsorbatos
- Modelamiento de la adsorcion sobre superficies y sistemas nanoscopicos
- Nano-diamantes y materiales superduros basados en carbono y carbono-silicio
- Desarrollo de templados nanoestructurados para la adsorcion enantioselectiva de especies quirales

Enantioselective Adsorption through Template Surfaces

Collaborating Groups:

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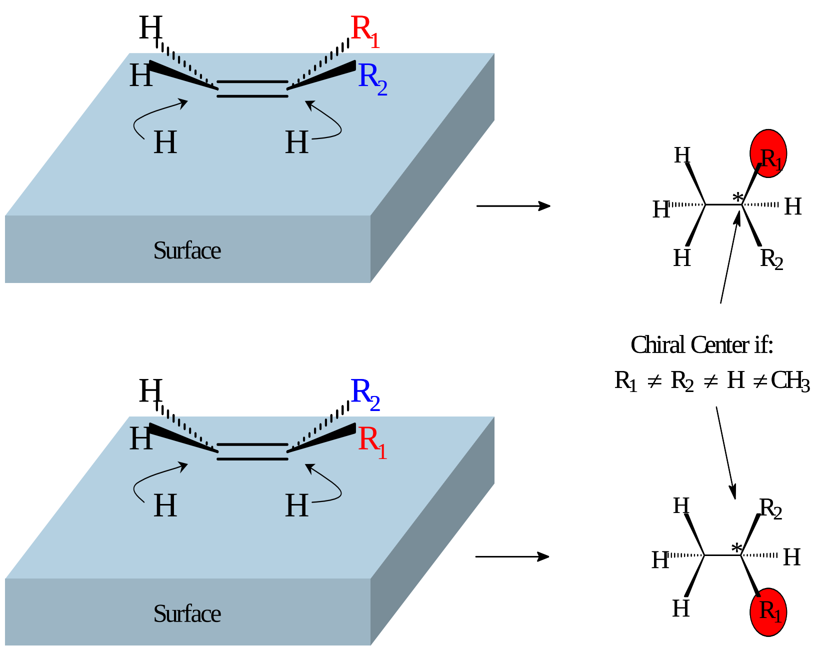
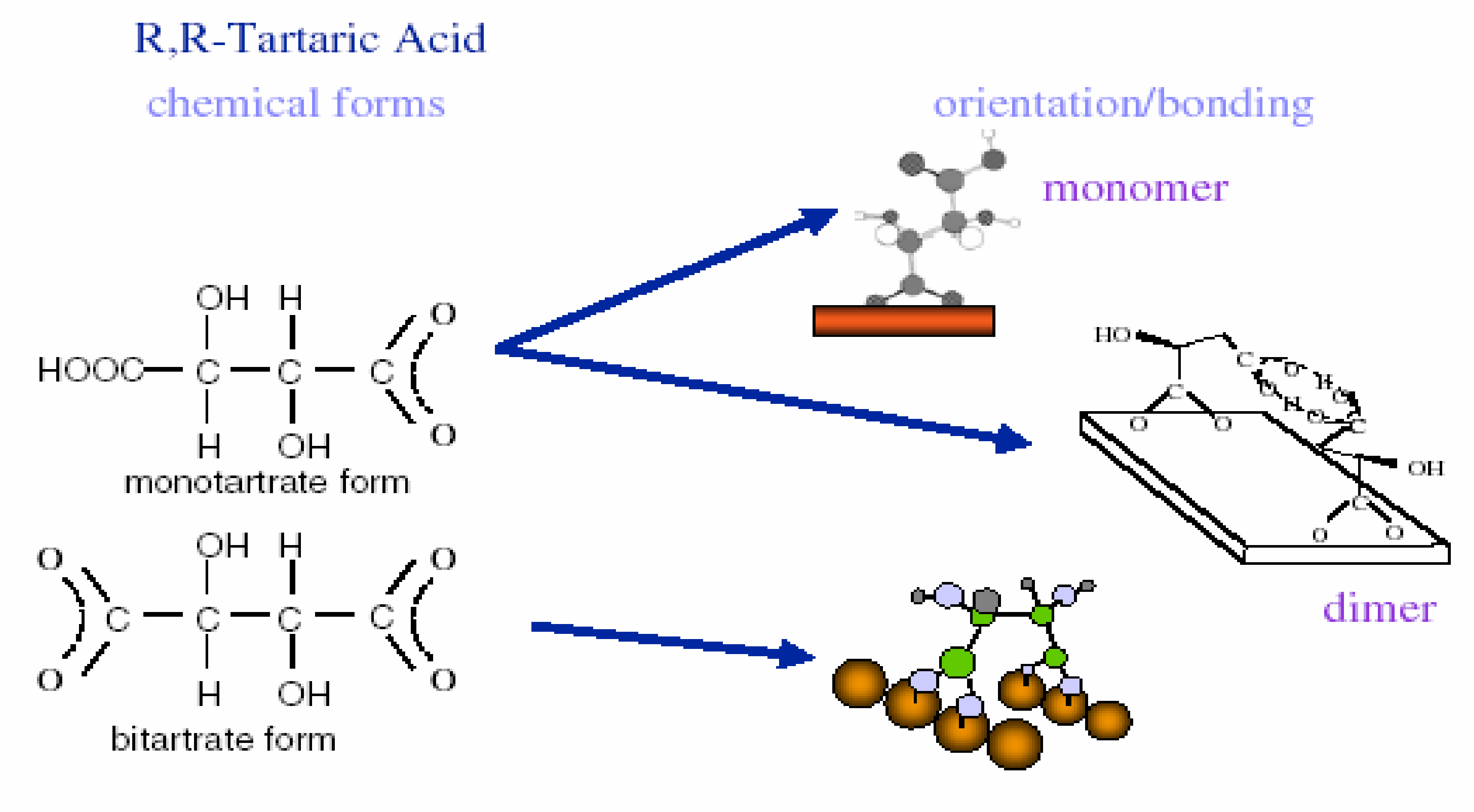
Objective



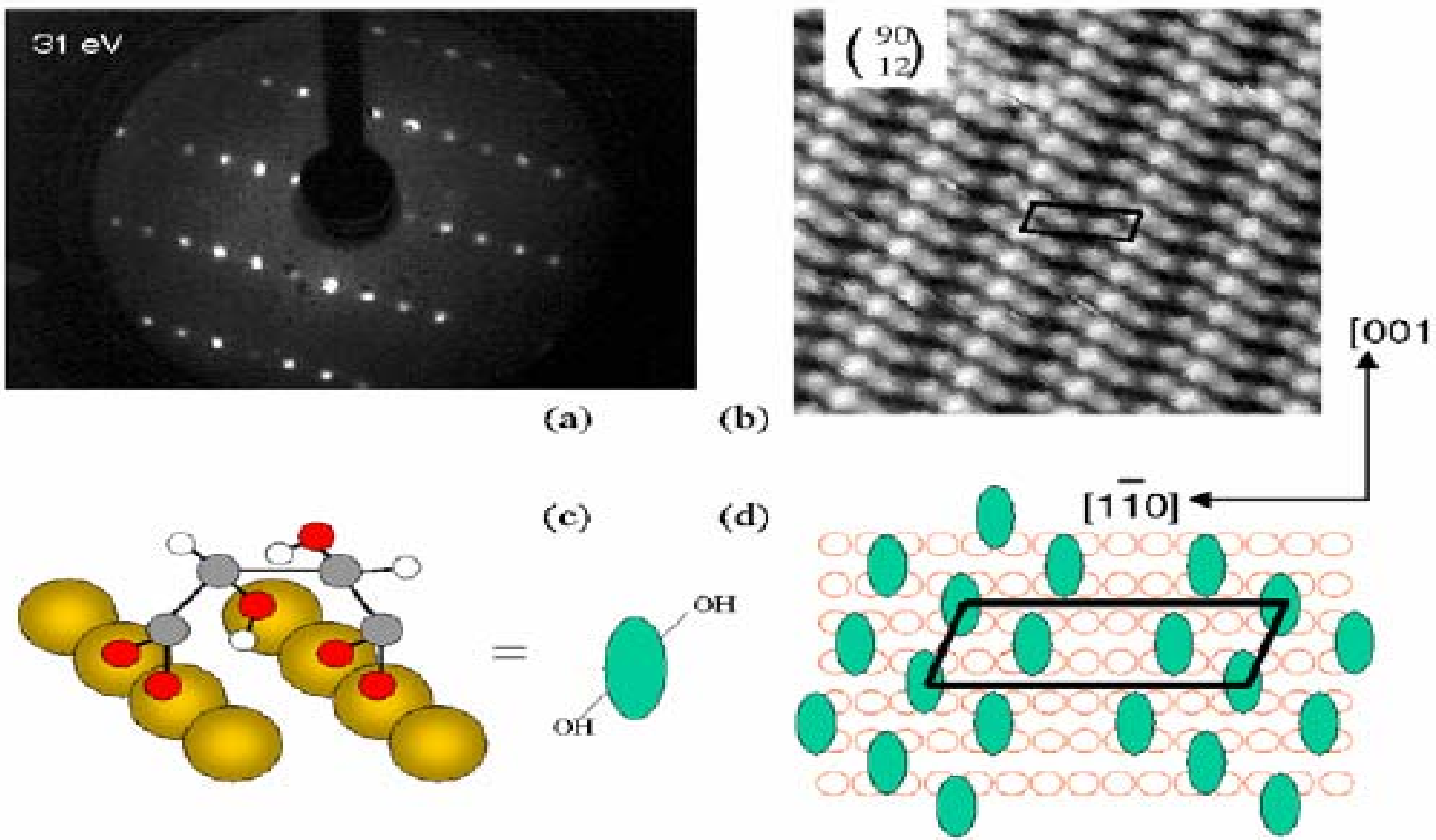
- Develop a surface capable of adsorbing preferently one of the two enantiomers of a chiral species
- Carry on the reaction obtaining an enantiomerically pure chemical
- Example: chiral hydrogenation

Surface Chiral Templates

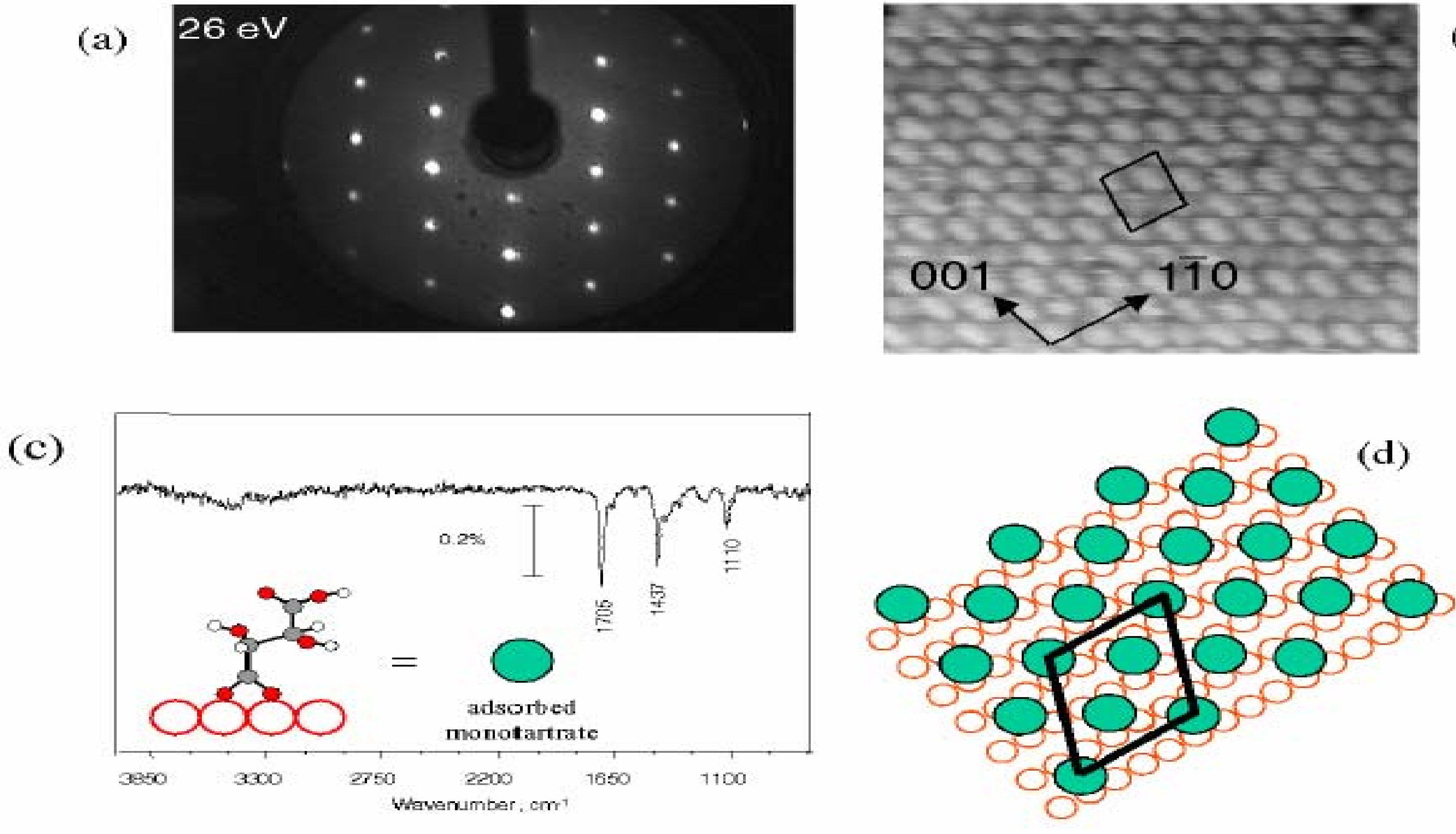
Tartaric Acid



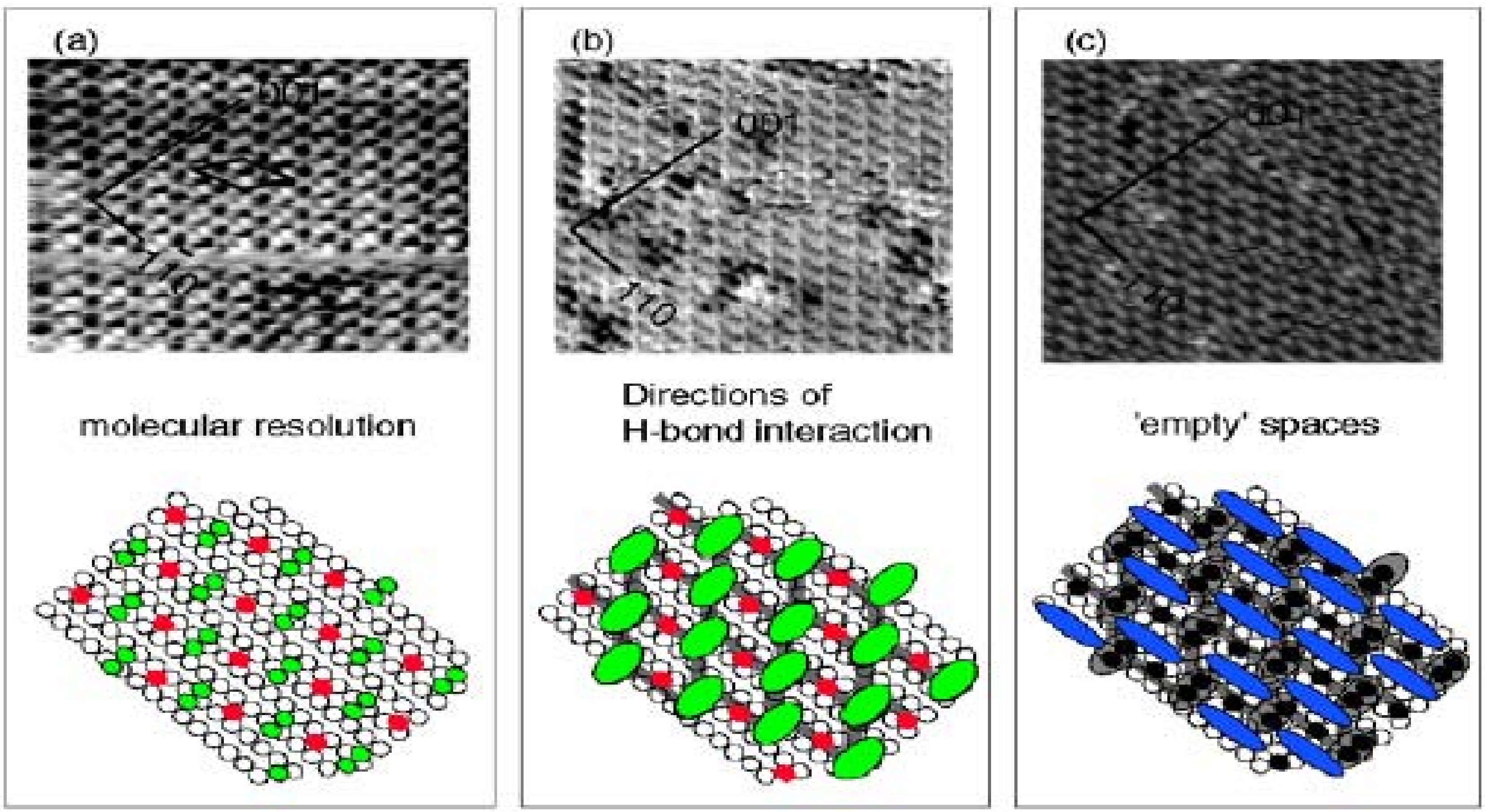
Low coverage: extended chirality



Middle coverage: no extended chirality



High coverage: extended chirality



Extended chirality → enantioselectivity

For extended chirality it is necessary:

- Chirality of template molecule
- Rigid and defined adsorption geometry
- Directional and anisotropic lateral interactions

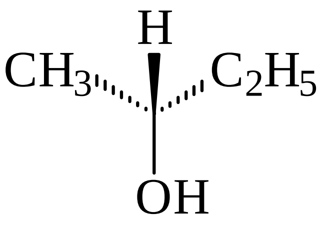
Selective adsorption of probe chiral species by chiral templates gives rise to characteristic sharp enantioselectivity peaks.

A Concrete example

2-butanol on Pd(111)

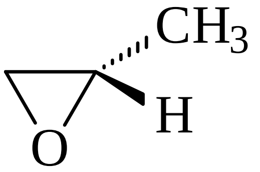
Experimental Strategy

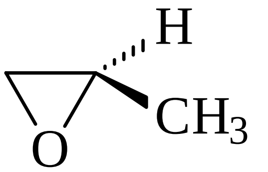
Adsorb chiral species onto the surface:



R-2-butanol

Probe chirality of the surfaces using propylene oxide:

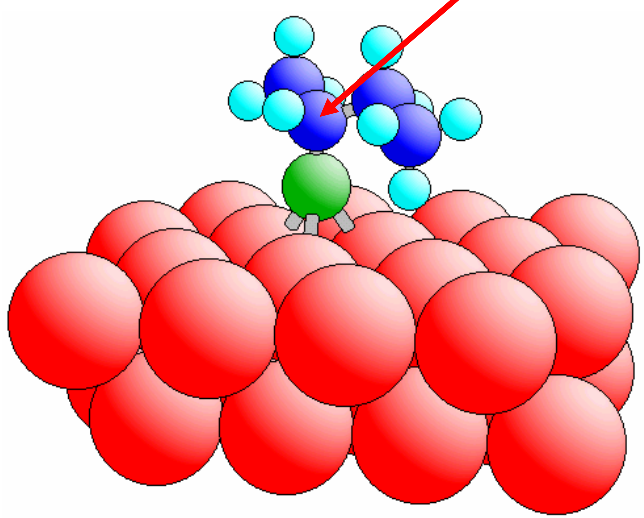




S-(-)-propylene oxide R-(-)-propylene oxide

Infrared Spectrum of 2-butanol on Pd(111)

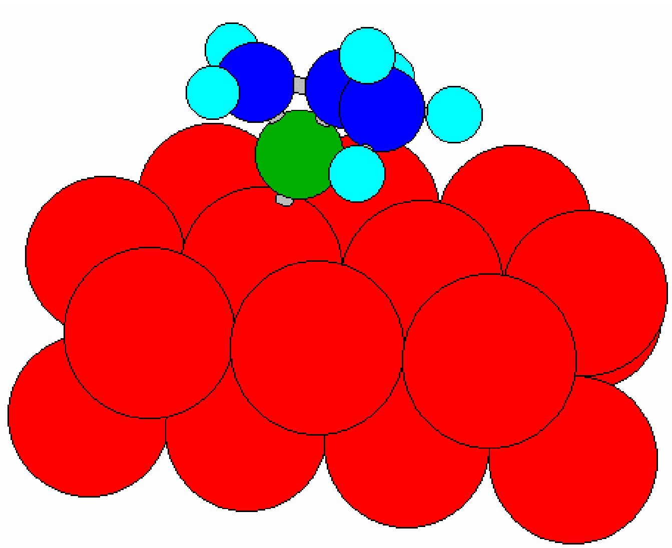
Chiral Center



$$C_2H_5CHOHCH_{3(ads)} \xrightarrow{Pd(111)}$$

$$C_2H_5C{=}OCH_{3(ads)}$$

Infrared Spectrum of Propylene Oxide on Pd(111)

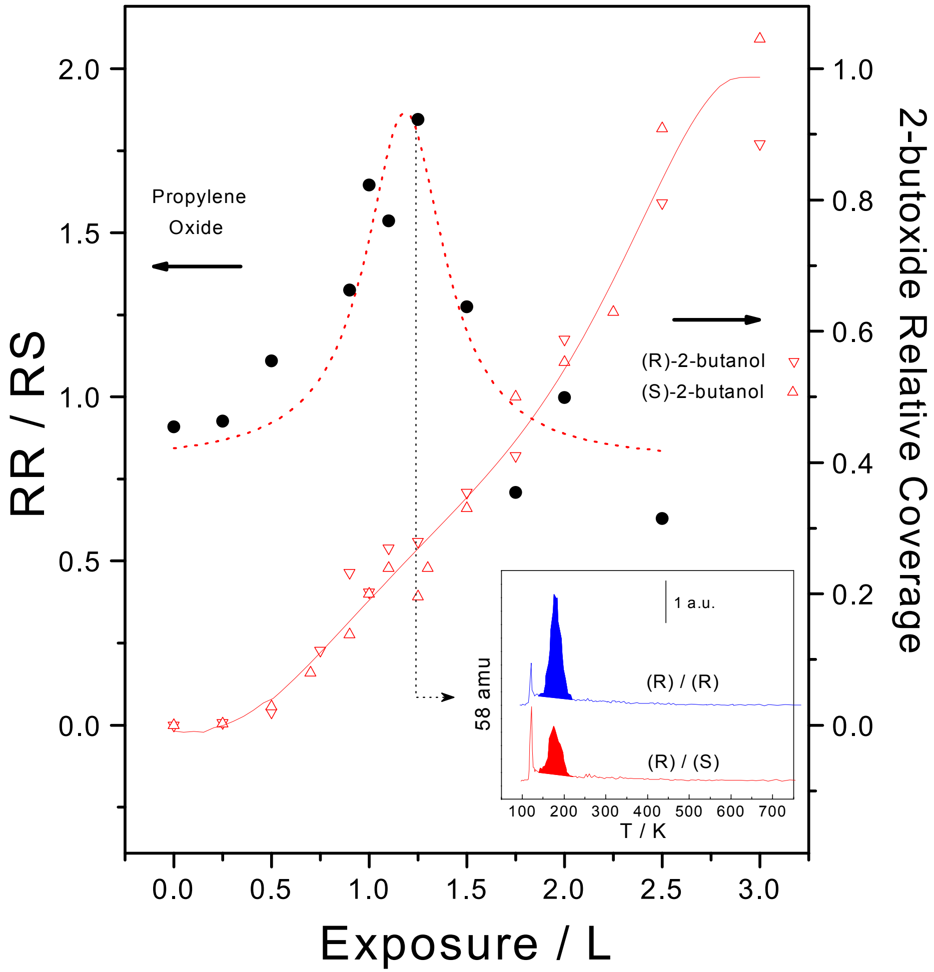


The monolayer and multilayer can be distinguished using infrared spectroscopy.

Multilayer

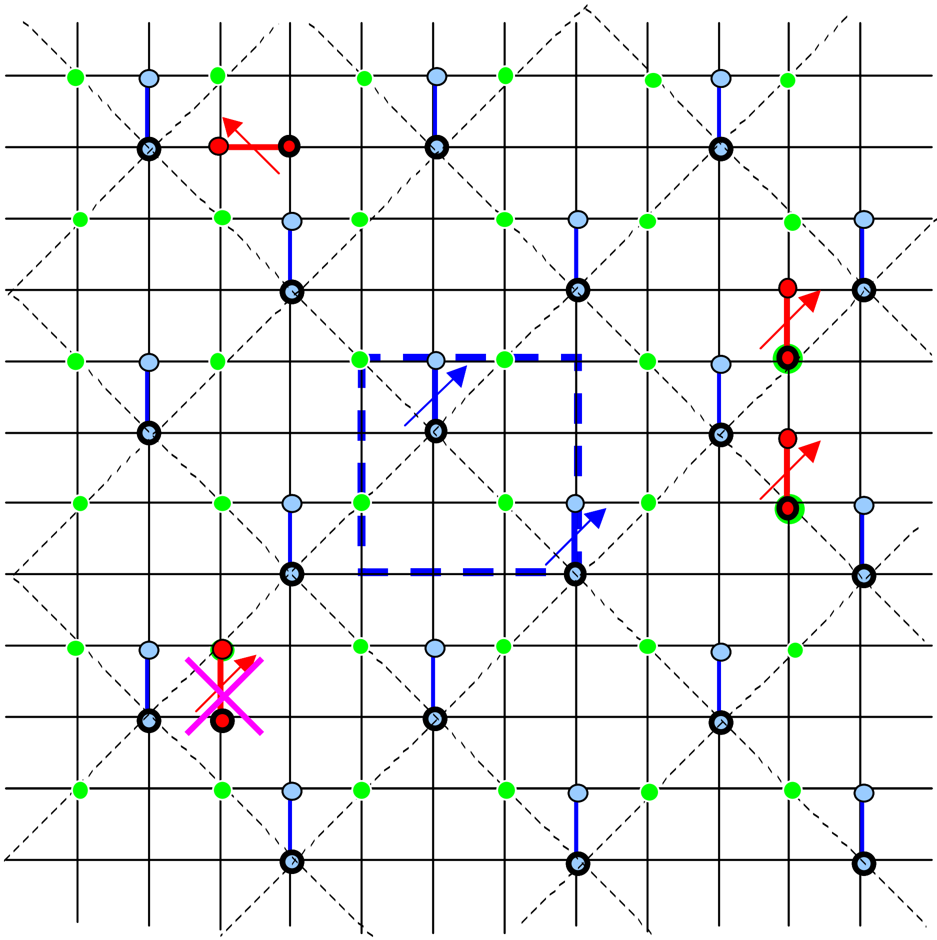
Monolayer

Enantioselective Adsorption of Propylene Oxide on 2-butanol/Pd(111) by TPD and RAIRS



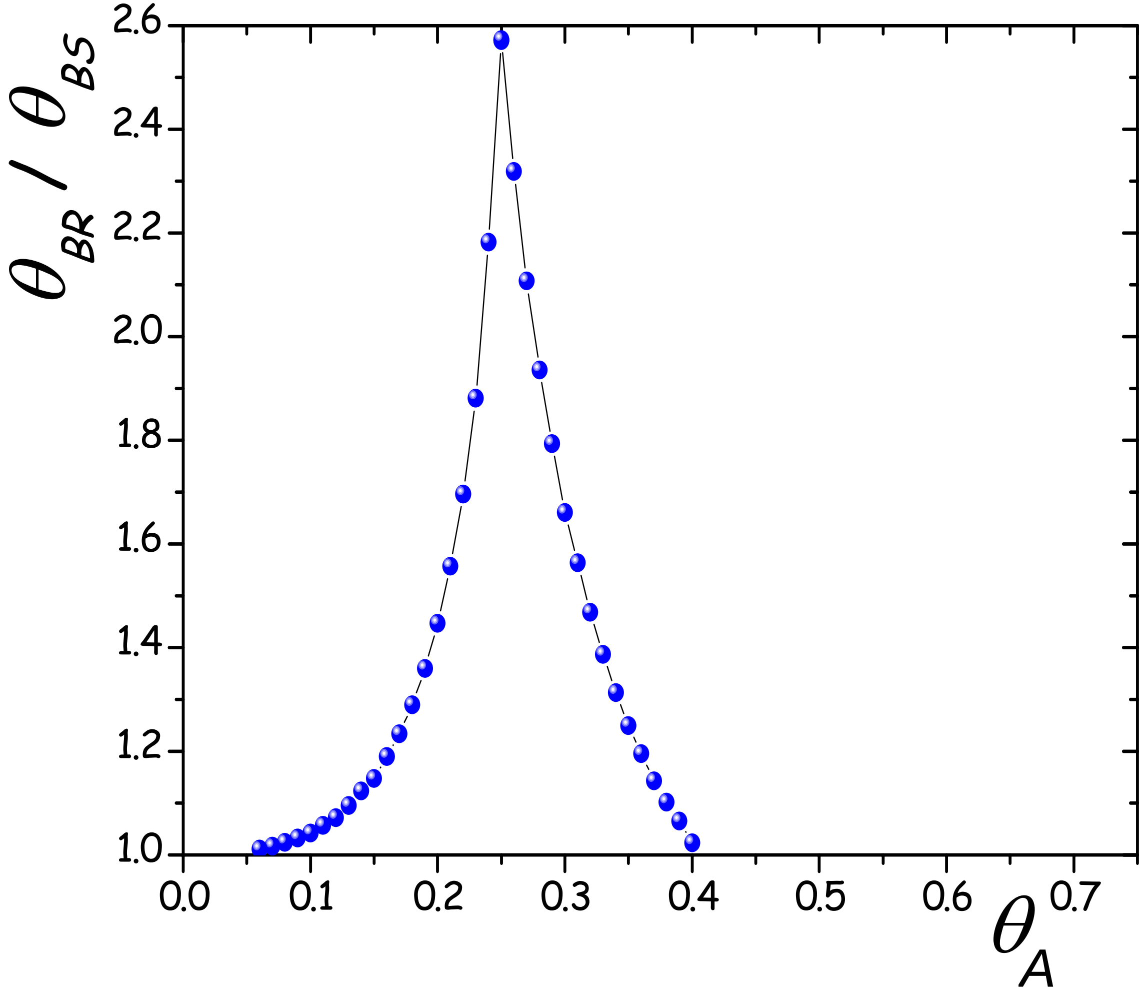
- **Enantioselectivity shows a sharp peak at a template coverage of approximately 0.25**

Modeling the Propylene Oxide (B) / 2-Butanol (A) System



- AR (blue dimers with arrow), coverage 0.25 ML; lower coverage obtained by random desorption; higher coverage by monomer adsorption on green sites.
- BR (red dimers with arrow), adsorb preferently on green sites.
- BS cannot adsorb on green sites between two adsorbed AR

Enantioselectivity of the model



Enantioselectivity shows a sharp peak at 0.25 coverage, in good concordance with experiments.