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New Methods for de Novo Simulations and Applications to Catalysis, Materials, and Biochemistry

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To solve the most challenging problems, we develop methods and software simultaneously. Current Focus

ARTIFICIAL PHOTOSYNTHESIS (JCAP) $H_2O + h\nu \rightarrow H_2 + O_2$,: HER, OER

ARTIFICIAL PHOTOSYNTHESIS (JCAP): $CO_2 + h\nu \rightarrow$ fuels: (MO/Cu); NP,

FUEL CELL CATALYST: Oxygen Reduction Reaction; Alkane fuels; Dealloyed

BATTERIES: Atomistic SEI-Li-IonicLiquid, anionic electrolytes, solid electrolytes

PEROVSKITES: MAPbI3, photoanodes, $BaTiO_3$, Ferroelectrics,

CERAMICS: Ductile ceramics, FC electrodes, FC membranes, HiTc

POLYMERS: Batteries (PEO) ; Fuel Cells electrolytes (Nafion, Anionic) BIOTECHNOLGY: GPCR Membrane Proteins, Pharma, GP activation

2D MATERIALS: MBE-graphene; MoS2, CVD, ALD

CATALYSIS: NH_3 synthesis, selective ammoxidation and oxidation alkanes

ENERGETIC MATERIALS: PETN, RDX, HMX, TATB, TATP, Propellants

COMBUSITION: Kinetics from full reaction reactive simulations

THERMOELECTRICS: (mechanical properties (brittleness))

Less active

SOLAR ENERGY: dye sensitized solar cells, CuInGaSe (CIGS/CdS) cells, Ionic Liquids

GAS STORAGE (H_2, CH_4, CO_2) : MOFs, COFs, metal alloys, nanoclusters

SEMICONDUCTORS: damage free etching

MultiParadigm Strategy: apply 1st principles to complex systems

Materials Design Requires Improvements in Methods to Achieve Required Accuracy. Our Focus:

1:Quantum Mechanics

Challenge: increased accuracy

- **New Functionals DFT** (dispersion)
- Meta Dynamics QM (DG† 298K)
- Accurate implicit solvation (CANDLE
- Grand Canonical QM (constant Potent
- Accurate Band Gaps

2:Force Fields

Challenge: chemical reactions

- **ReaxFF and RexPoN- Describe Chemical Reaction processes**, Mixed Metals, Ceramics, Polymers
- Accelerated Reactive Dynamics
- **NonEquil QM Dynamics** (eFF)
- Hybrid QM-ReaxFF

3:Biological Predictions

1st principles structures GPCR-GP acti

1st principles Ligand Binding

Conditional siRNA therapeutics

4: Molecular Dynamics

Challenge: Extract properties essential to materials design

- Non-Equilibrium Dynamics
  - Viscosity, rheology
  - Thermal Conductivity
- Plasticity, Dislocations, Crack
- Interfacial Energies
- surface tension, contact angles
- Reaction Kinetics
- Entropies, Free energies
- surface tension, contact angles

5: Coarse Grain Reactive MD

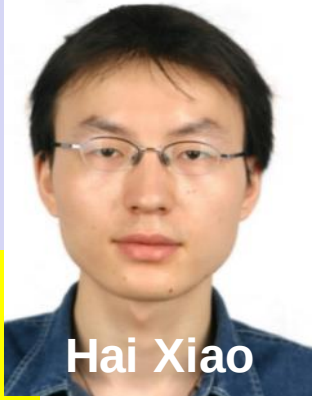
6: Integration: Computational Materials Design Facility (CMDF)

- **Seamless across the hierarchies of simulations using Python-based scripts**

Need new theory methods to solve key problems in energy and environment

Grand Canonical QM (constant potential not constant electron as usual with QM)

Traditional QM calculations use a fixed number of electrons. But in electrocatalysis, the potential at the electrode is kept constant during the electrocatalysis

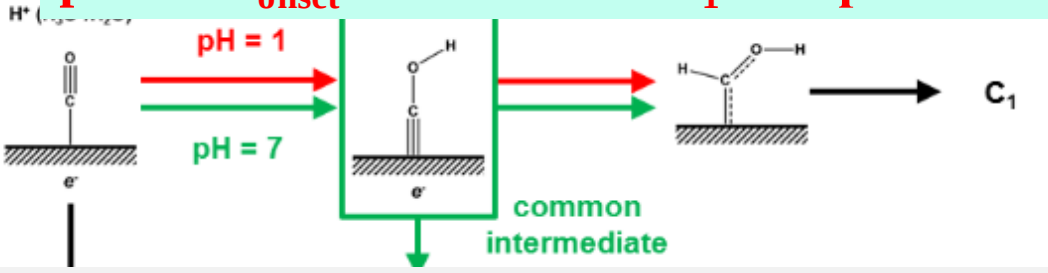


Methods for Grand Canonical QM now worked out. Onset potentials within 0.05V for Cu(111), all pH

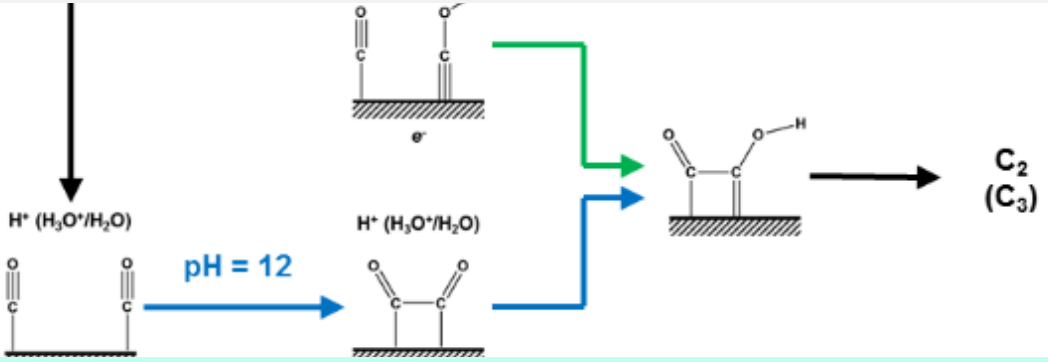
pH Dependence and Onset Potentials for Hydrocarbon Products from Electrochemical Reduction of CO on Cu (111); Xiao, Cheng, Goddard, Sundararaman; J. Amer. Chem. Soc., 138 (2). pp. 483-486 (2016)

Grand canonical electronic density-functional theory: Algorithms and applications to electrochemistry Sundararaman, Goddard, Arias. J. Chem. Phys. (2017) 146 (11). Art. No. 114104.

pH=1: U_{onset} = −0.80 V for C_1 *vs* expt. −0.76 V

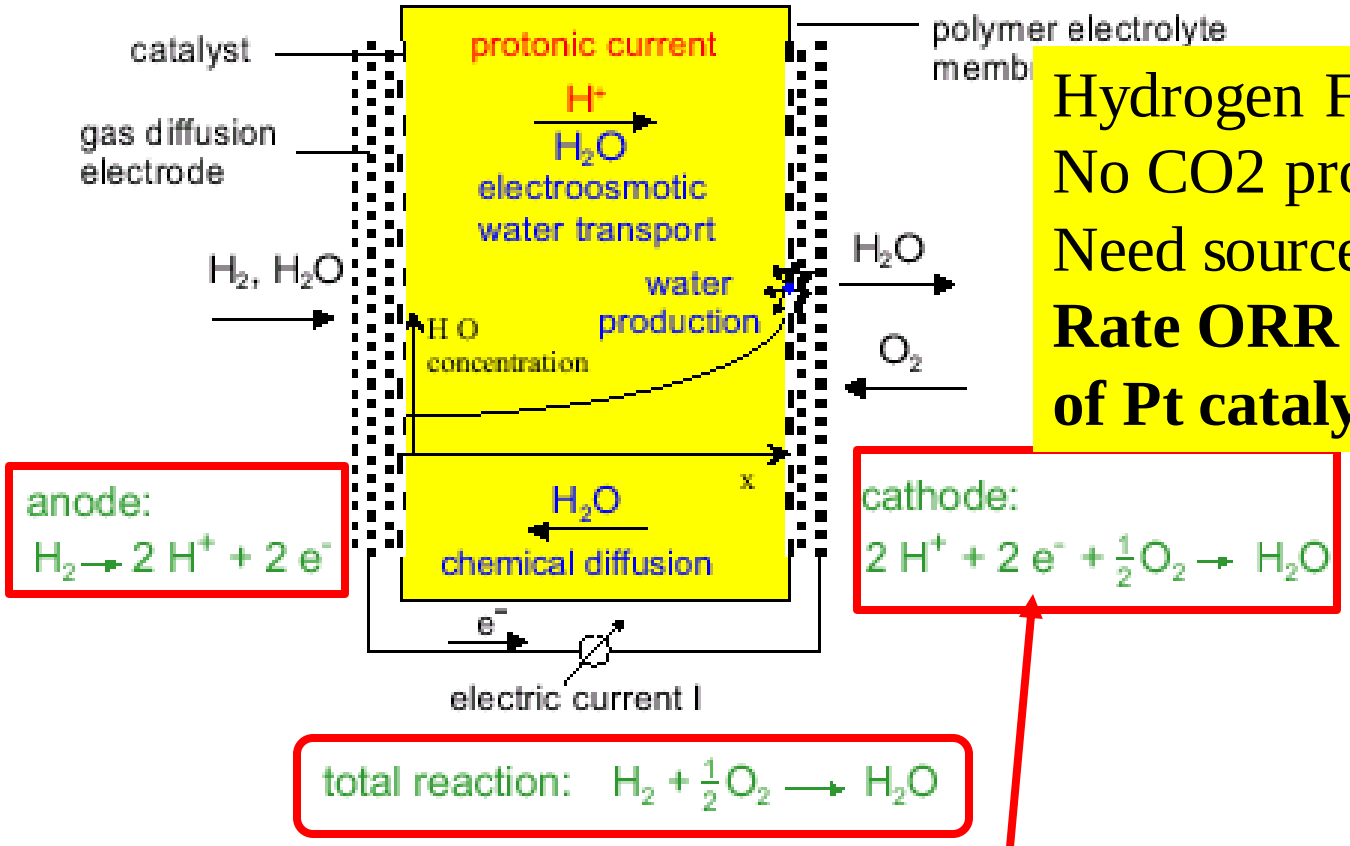


pH=7: U_{onset} = −1.17 V for C_1 and C_2 *vs* expt. −1.20 V



pH=12: U_{onset} = −1.21 V for C_2 *vs* expt. −1.26 V

Kinetics of the Oxygen Reduction Reaction on Pt(111) from Ab initio Molecular Dynamics Free Energy Calculations at 298 K including explicit solvent

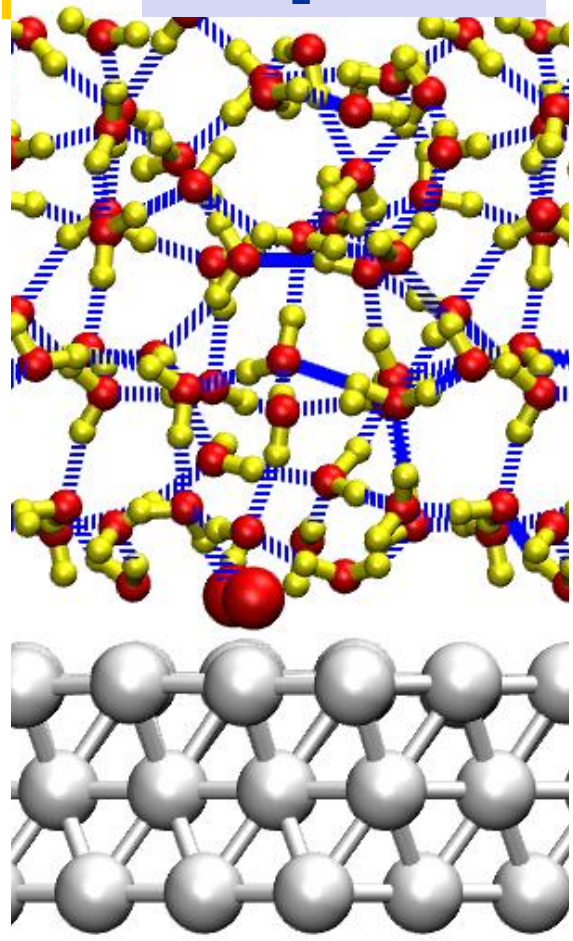


Hydrogen Fuel Cell
No CO2 products
Need source of H2
Rate ORR too slow➔ Expense of Pt catalyst too high

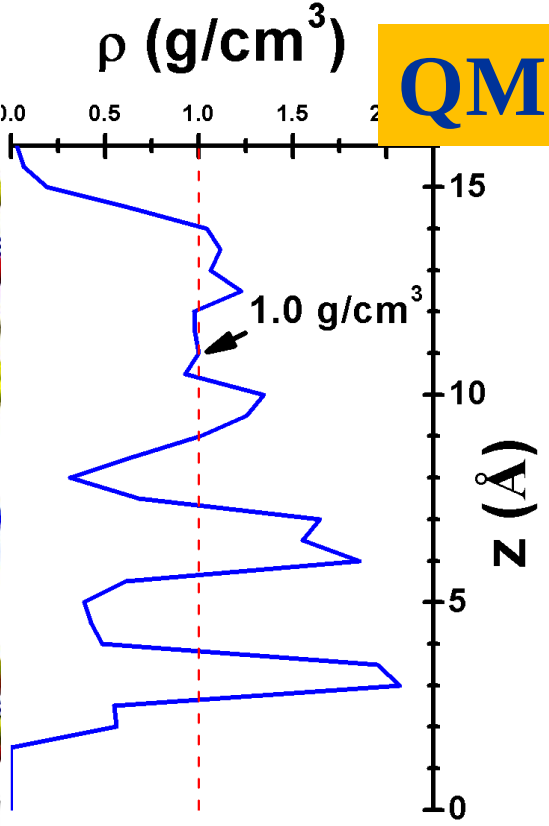
Oxygen Reduction Reaction (ORR)
Proton from anode + O2 at cathode ➔ H2O
Currently ~400 times slower than the anode reaction

QM metaMD full solvent

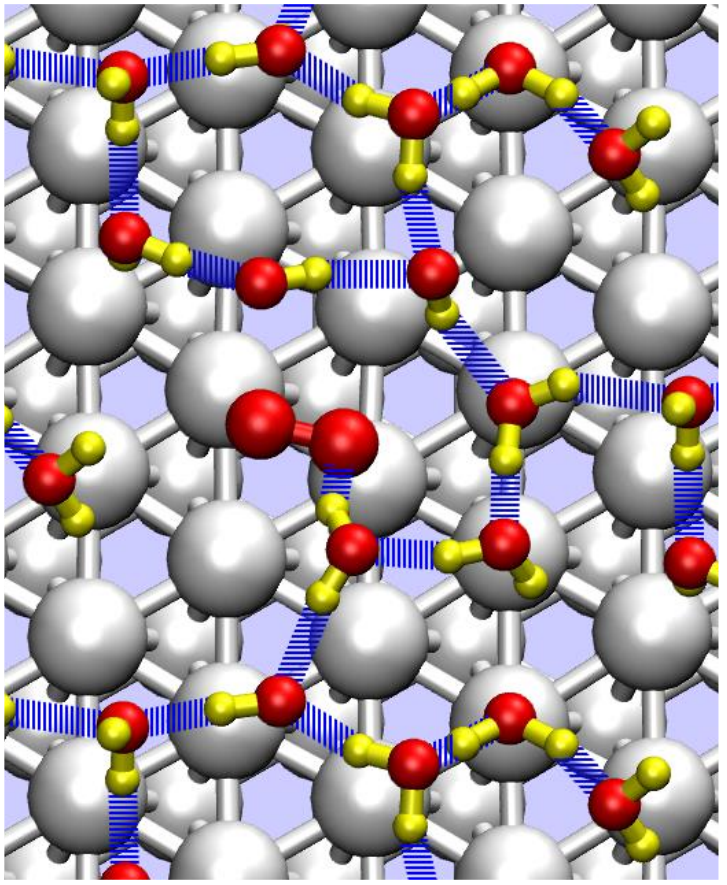
A 5 layers H_2O
50 H_2O



Side view of Surface structure of water/Pt(111) interface



water density distribution (center of mass) perpendicular to the surface (z direction),



first contact layer of water from top view Pt(111) 4x4 unit cell

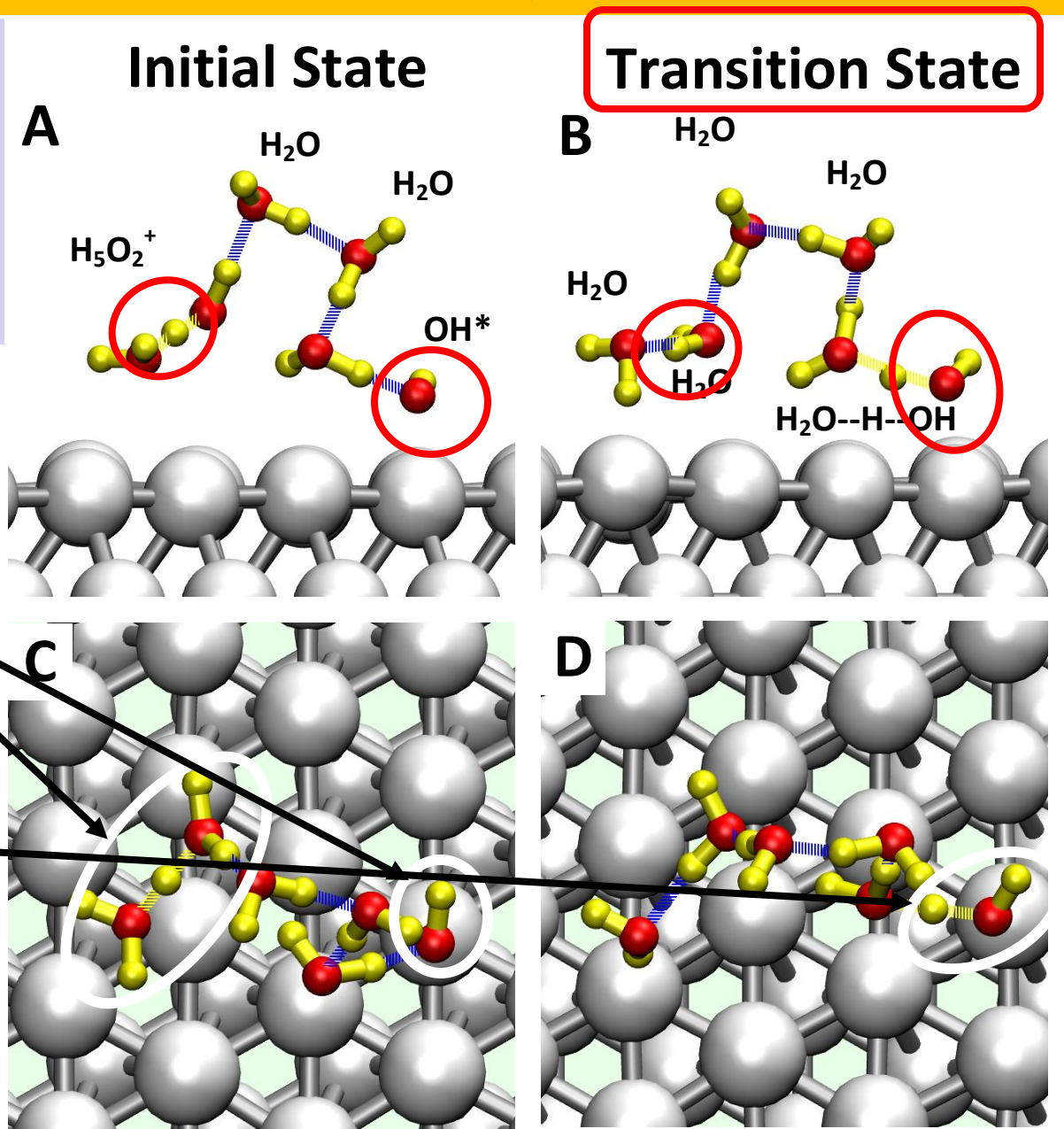
Snapshots of structures during for water formation. $H_3O^+ + e^- + OH^* \rightarrow 2 \cdot H_2O$)

0.6 V potential with one extra H_3O ($H_3O^+ + e^-$)
Initial state
Water molecules not involved are hidden, for viewing convenience.

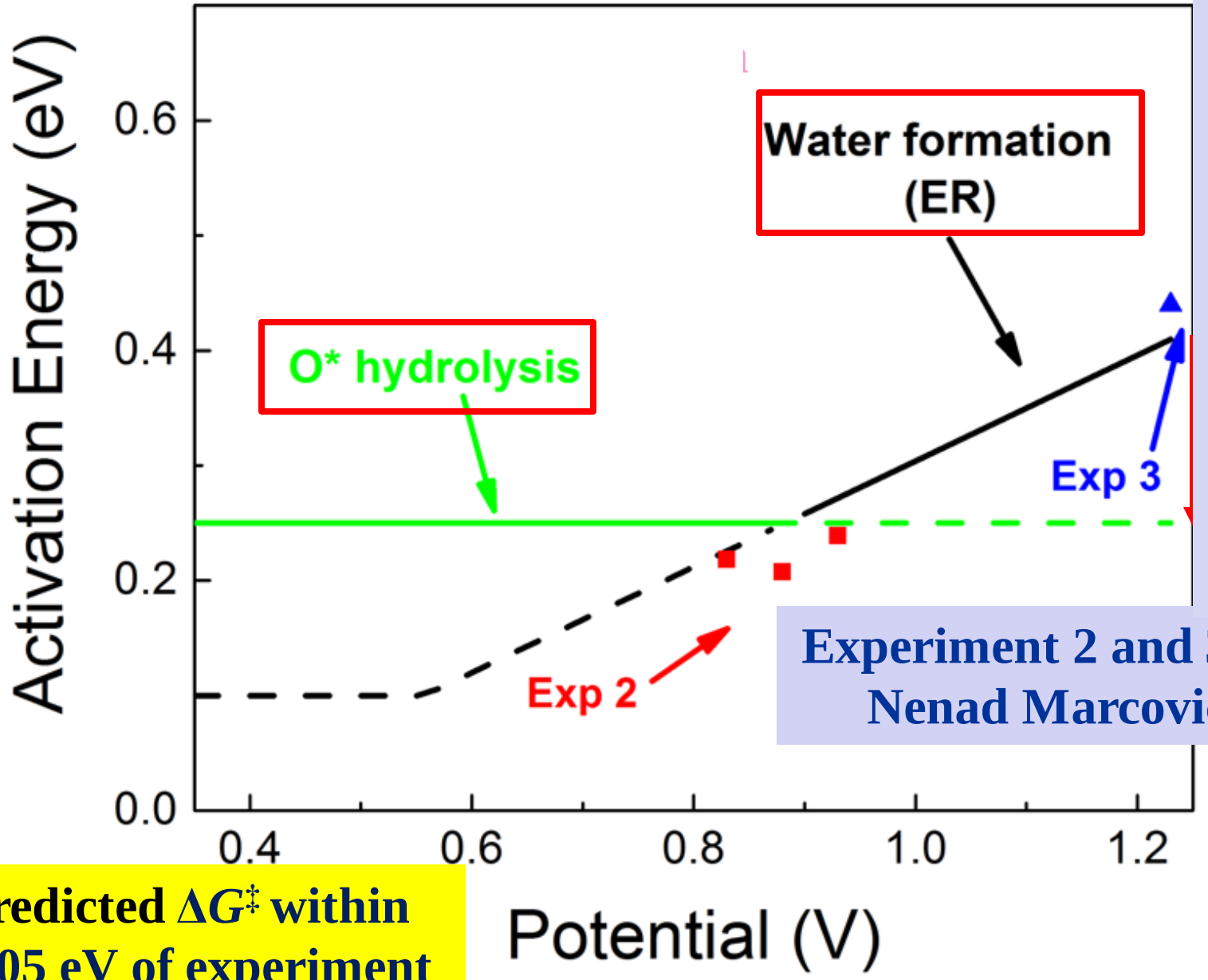
The reaction starts with one $H_5O_2^+$ complex and one OH*.
Three intermediate water molecules are involved in proton tunneling (Grotthuss mechanism)

Product H2O

The colors of atoms are:
Pt in silver, H in white, and O in white.



Predicted $\Delta G^{\ddagger}$ in eV for the rate determining steps from full solvent DFT calculations at various applied potentials,

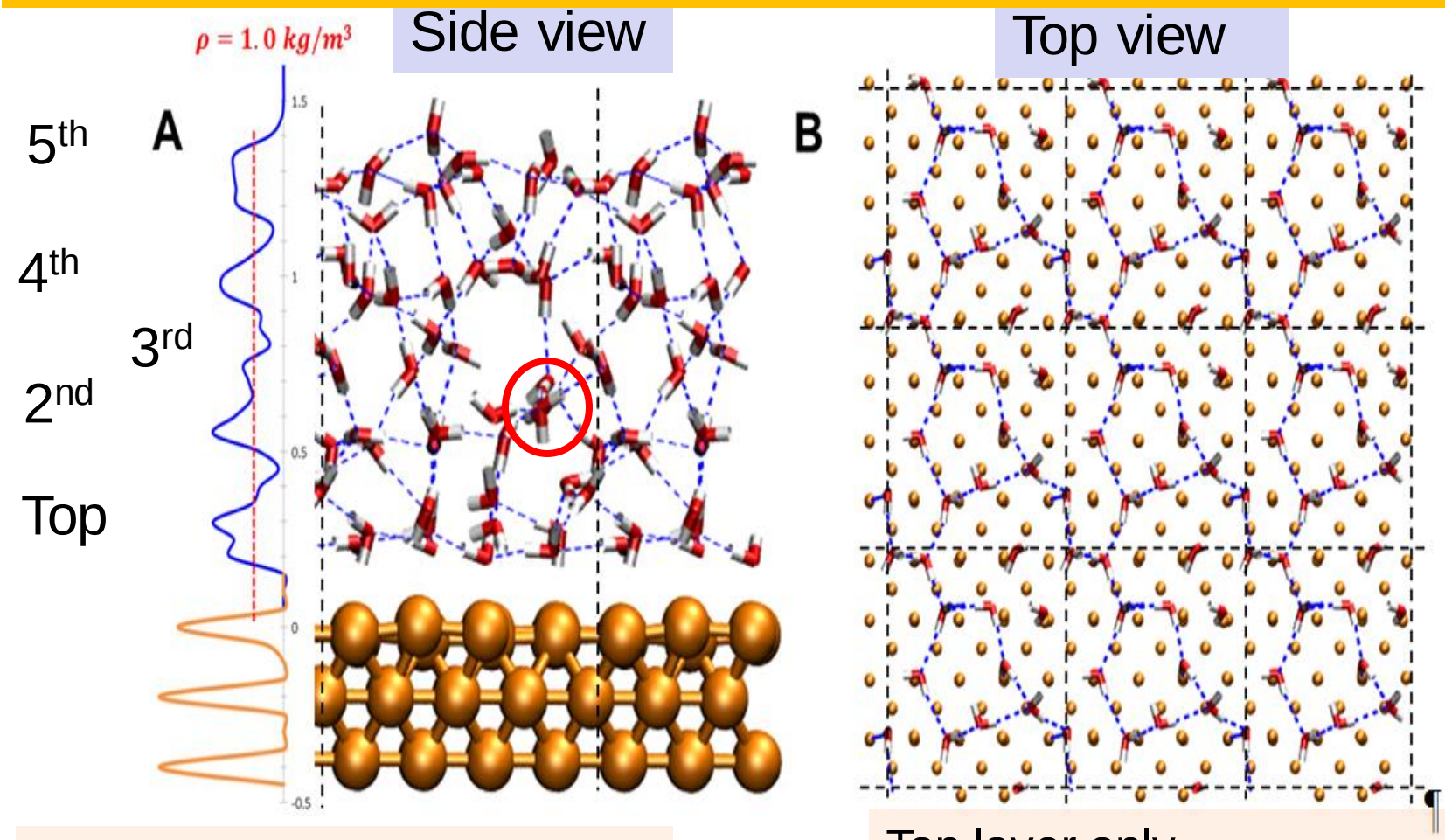


If we could decrease $\Delta G^{\ddagger}$ from 0.42 to 0.25 at 1.2 V Rate would increase by factor of 600 Even factor of 6 make PEMH2 Fuel Cell for autos practical

Experiment 2 and 3 in water
Nenad Marcovic, ANL

Predicted $\Delta G^{\ddagger}$ within 0.05 eV of experiment

activation of CO2 with full solvent QM metadynamics on Cu(100) the stable surface under electrochemical conditions



Cu 3 layers 4x4, 48 atoms
49 H2O, one is H_3O^+ ➔ pH=0
One H* and 2 CO*

Top layer only
12 H_2O; 16 sites; ¾ ML

Water/Cu(100) first layer

Observe a loosely packed hydrogen-bond network.

ΔG‡ rates for QM-metaMD for CORR on Cu(100) at pH=7

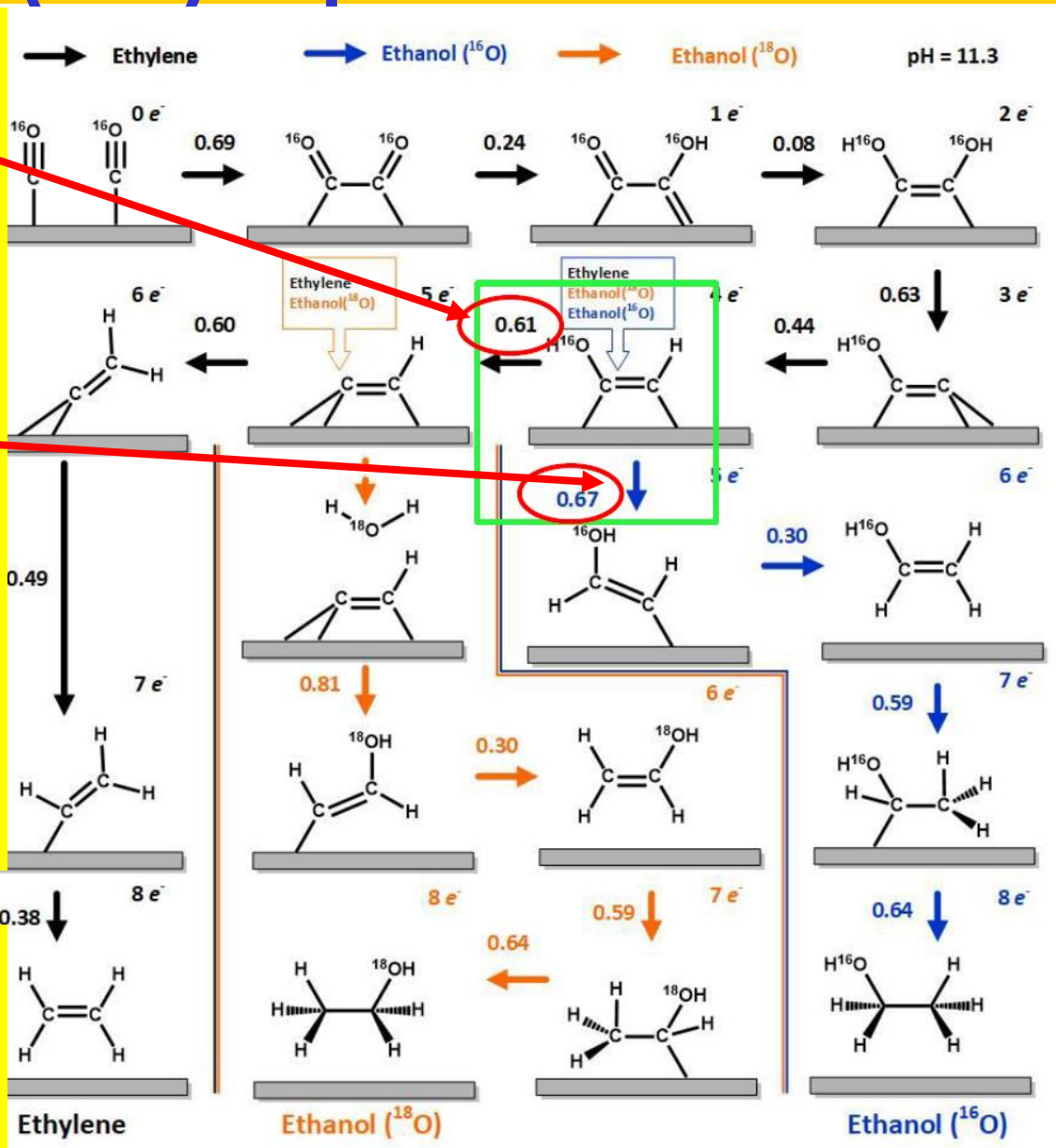
QM-metaMD barrier ΔG‡=0.61 eV to form *C-CH is (red circle) leads to ethylene and ^{18}O ethanol.

QM-metaMD barrier ΔG‡=0.67 eV to form *H(^{16}OH)C-CH (red circle) leads to ^{16}O ethanol.

This ΔG‡=0.06 eV➔ratio of 11:1

experimental ratio =14 ➔ 0.066 eV (Lum, Agar)

Thus QM-metaMD distinguishes partitioning between pathways within 0.01 eV



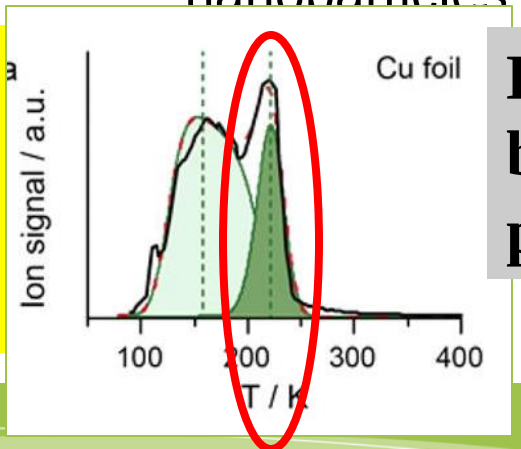
We now understand from QM on 200 atom systems the Reaction mechanism on low index surfaces
But Nanoparticle and Nanowire catalysts often lead to dramatic improvements.

- Cu nanoparticles (NPs) can **reduce CO at potentials ranging from -0.3 V to -0.5 V (RHE)** reaching a mass activity of up to ~1.5A per gram of Cu and a Faradaic efficiency > 70% at -0.3 V;
- CO reduction correlates with the **density of grain boundaries (GBs)** in Cu NPs.

Concludes: Grain Boundaries are responsible for creating the vast majority of the active surfaces.

TEM characterization of Cu nanoparticles in the Cu/CNT

10-20 nm NP ➔ 200,000 atoms
How can we apply our now validated QM methods to these systems? Answer ReaxFF



High CO binding ➔ High performance

Feng et al. *ACS Cent. Sci.* 2016, 2, 169-174

mechanism (100)
Nanoparticle and Nanowire catalysts dramatic

Typical NP is 10-20nm ➔ 200,000 atoms
How can we apply our now validated QM methods to these systems?

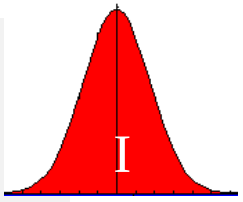
For systems too large for QM (>1000 atoms) ReaxFF reactive force field ➔ energetics similar to QM but 10**6 times faster

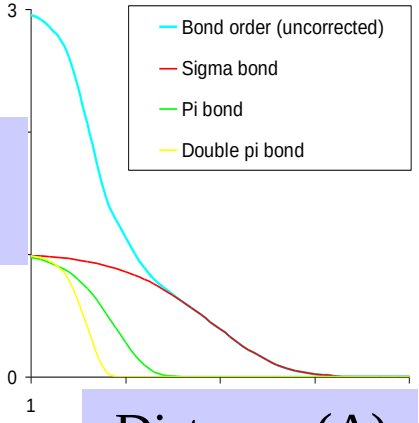
$$E = E^{Val} + E^{Coul} + E^{VdW}$$

Valence energy

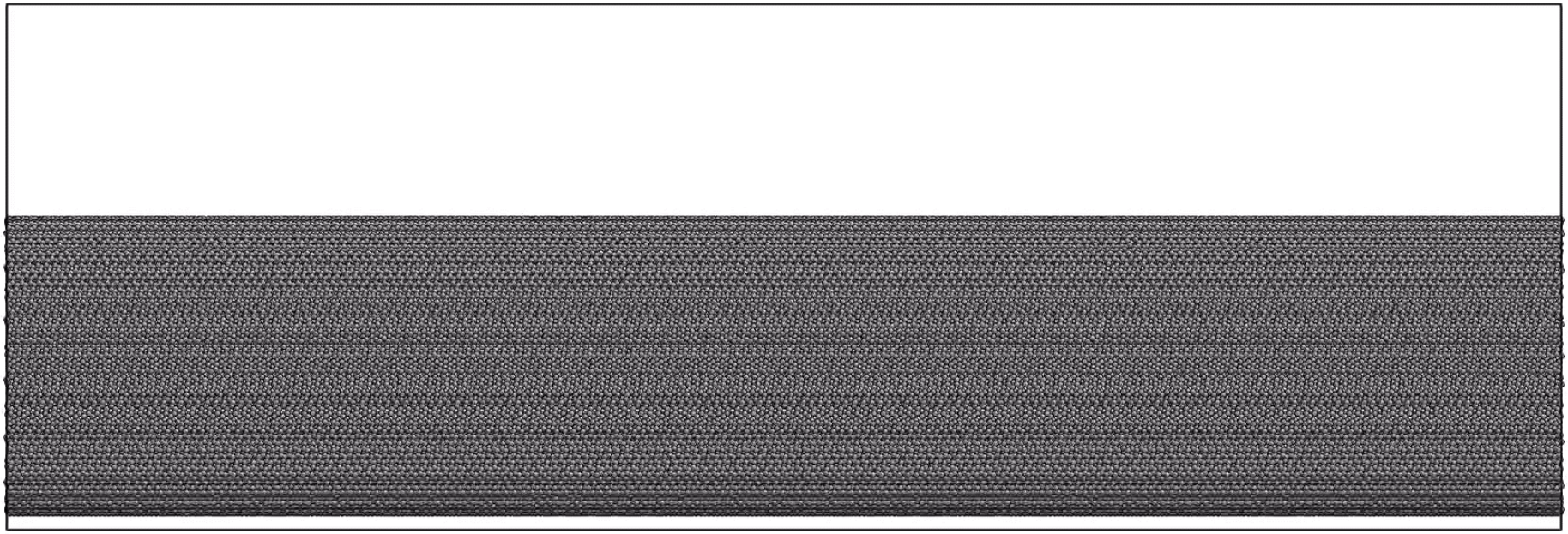
Electrostatic energy

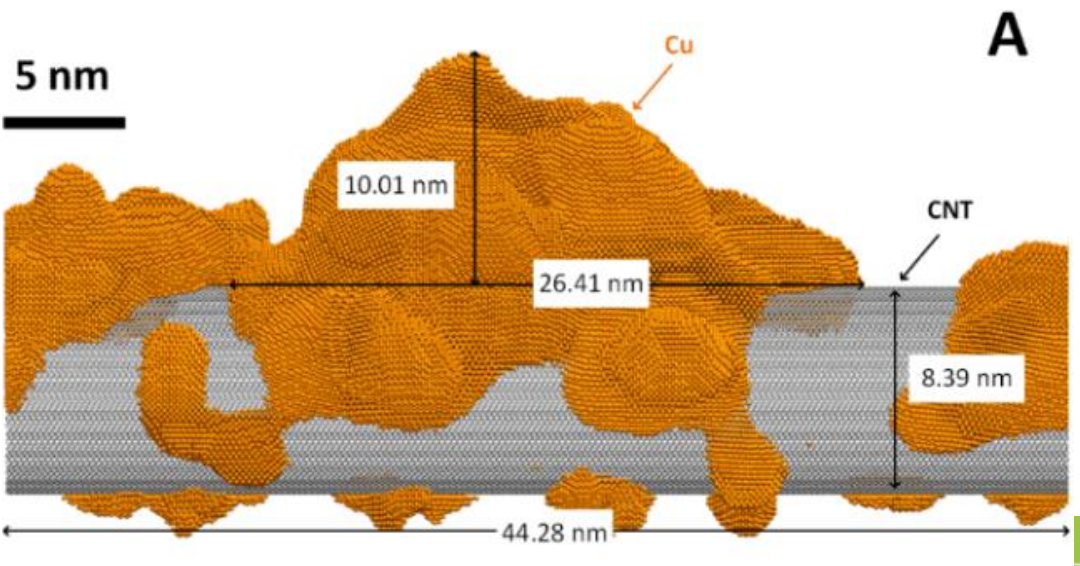
- Self-consistent Charge Equilibration (QEq)
- Finite Gaussian shaped charge size of atom
- Allow charges to transfer as reactions occur

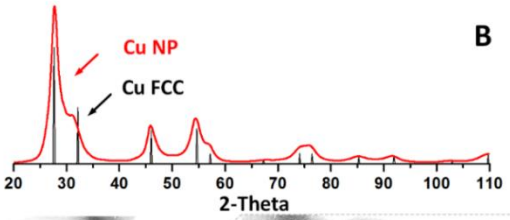


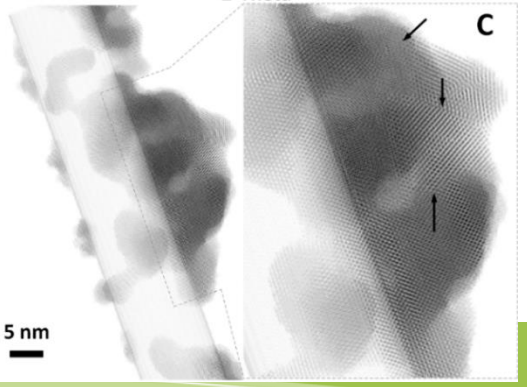


Computationally growth a Cu nanoparticle using Reactive force field







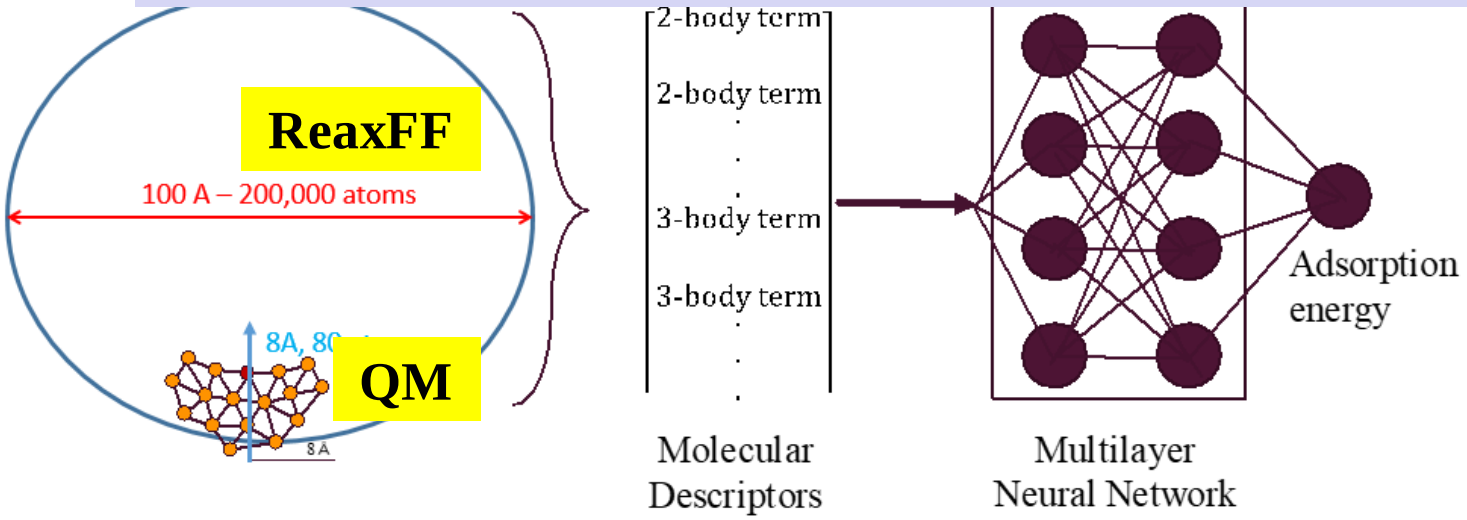


JCAP
JOINT CENTER FOR ARTIFICIAL PHOTOSYNTHESIS

Problem 10nm NP ➔200,000 atoms 10,000 surface sites

How can we be sure to find best sites
Need fast way to predict binding at all 10,000 sites

Use *Neural Network Machine Learning Model*



Analyze 400 surface sites in terms of two-body and three-body neighbors

$$G_{i\alpha}^{(2)} = \sum_j \phi_\alpha^{(2)}(\boldsymbol{p}_{ij}) \cdot ; \cdot G_{i\beta}^{(3)} = \sum_{jk} \phi_\beta^{(3)}(\boldsymbol{p}_{ij}, \boldsymbol{q}_{ijk}) \cdot \cdot$$

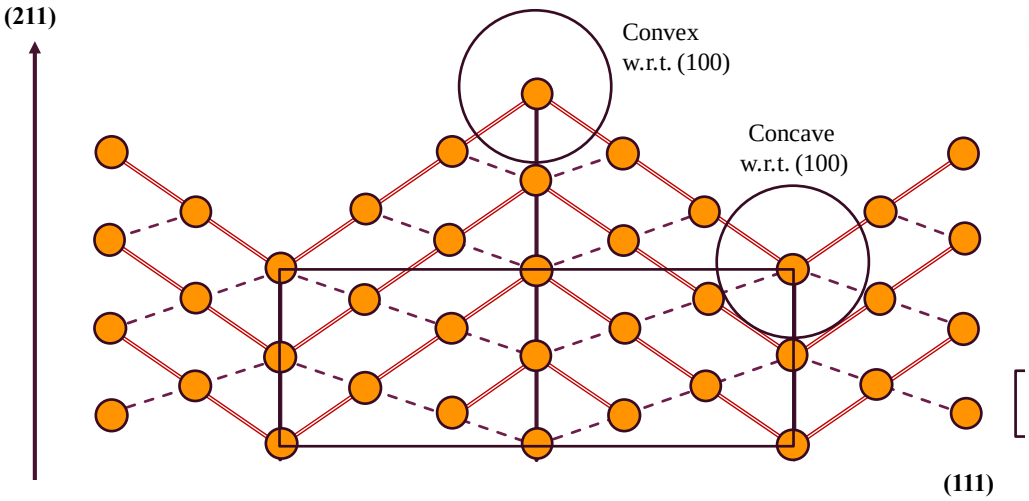
$$E_{CO} = F_{NN}\left(\left\{G_{i\alpha}^{(2)}, G_{i\beta}^{(3)}\right\}; \boldsymbol{w}, \boldsymbol{b}\right) \cdot$$

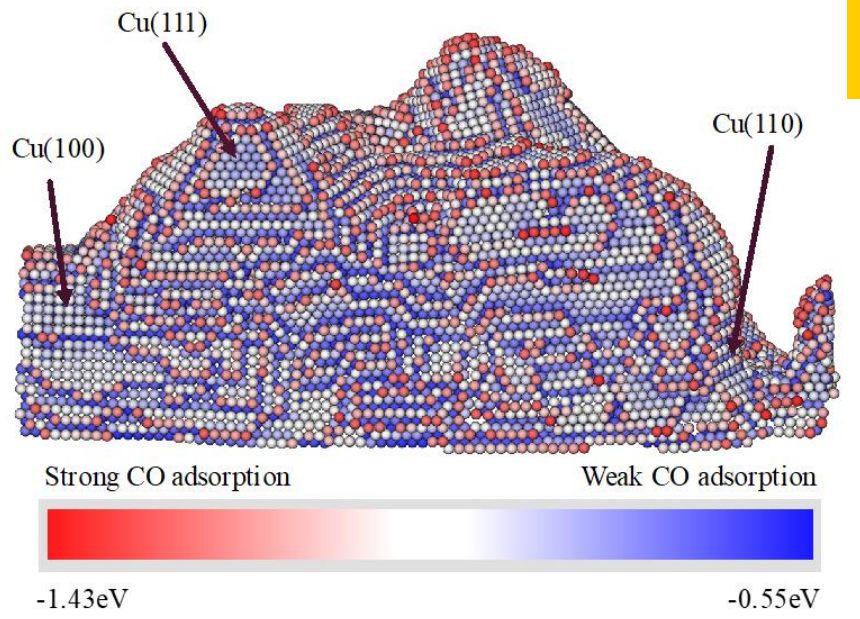
E_{CO} predicted adsorption energy

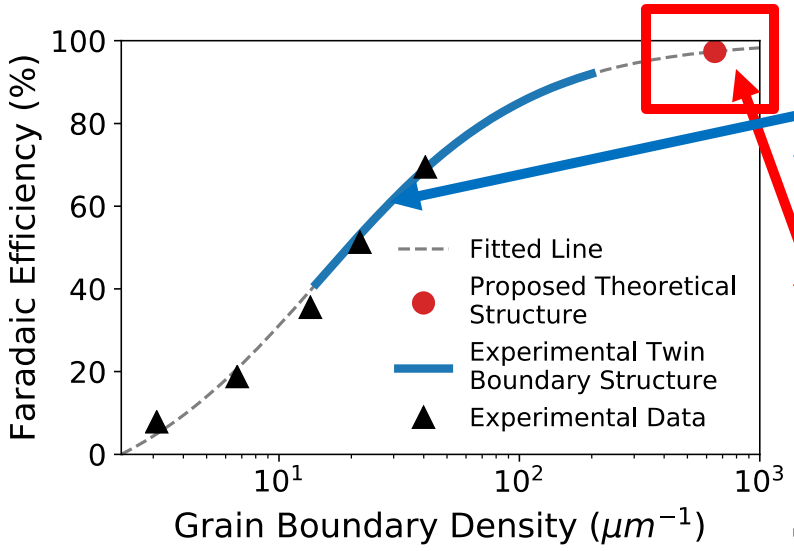
network network transforms input descriptors G into single values & weights w, biases b.

2-body descriptors 3-body descriptors

Designed periodic structure with optimum twin boundary







Extrapolated faradaic efficiency (FE) of the concave site on the minimal periodic structure using experimental data.

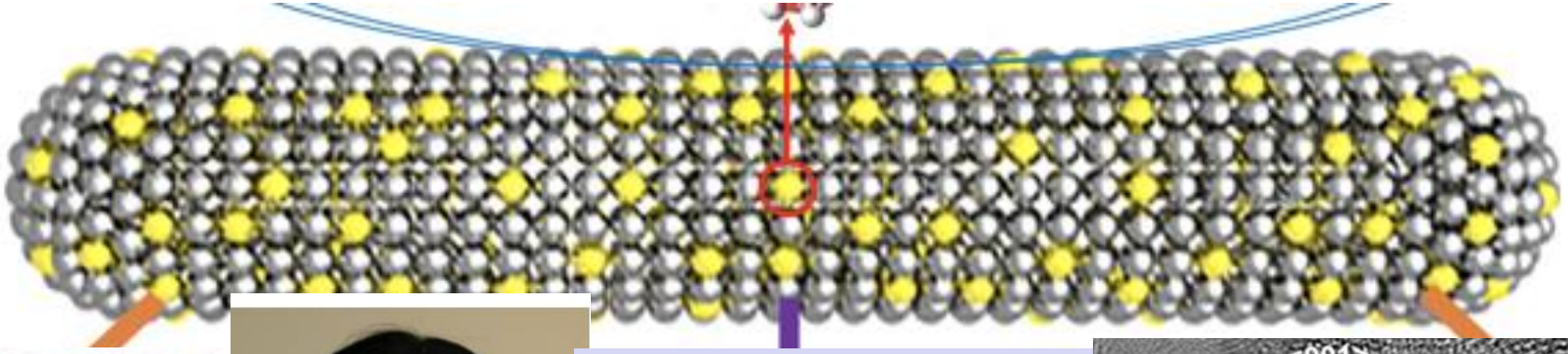
Predicted copper structure with maximized twin boundaries extrapolated based on the densities of the boundaries.

Next do full solvent QM on predicted structure to validate.

Then use ReaxFF to develop same structure with Atomic Layer Epitaxy with Au and Fe lines

Problem with previous OER predictions
Structure is not known, we assume γ-NiOOH

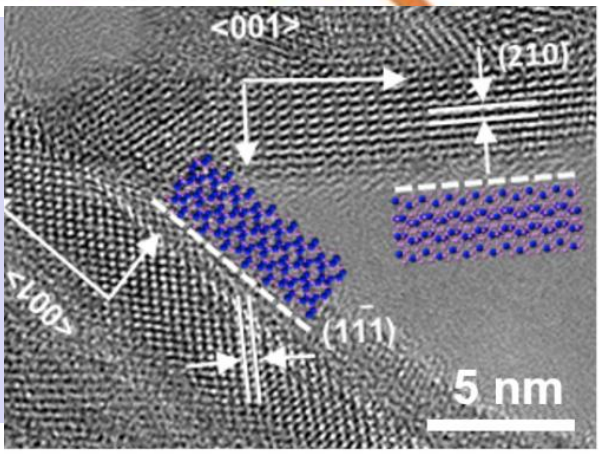
Sen Zhang U. Virginia: Single Atom Doped TiO2 uses organic solution colloidal synthesis ($TiCl_4$ precursor, C_{18} surfactants (oleylamine, OAm; oleic acid, OAc) and 1-octadecenorganic solvent] to Get single crystal Brookite structure with {210} surface square cross-section. EXAFS, XAS ➔ no Co-Co neighbors



Sen Zhang
U. Virginia

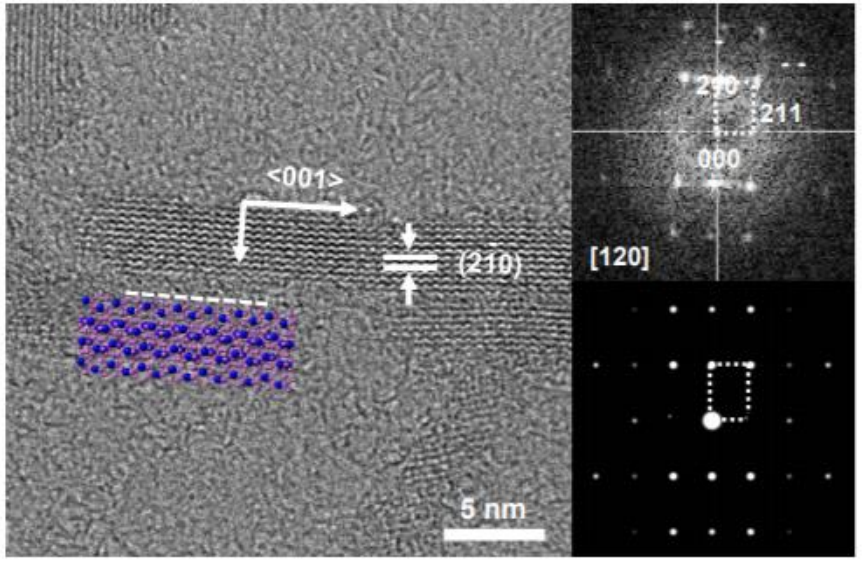
Jin Qian

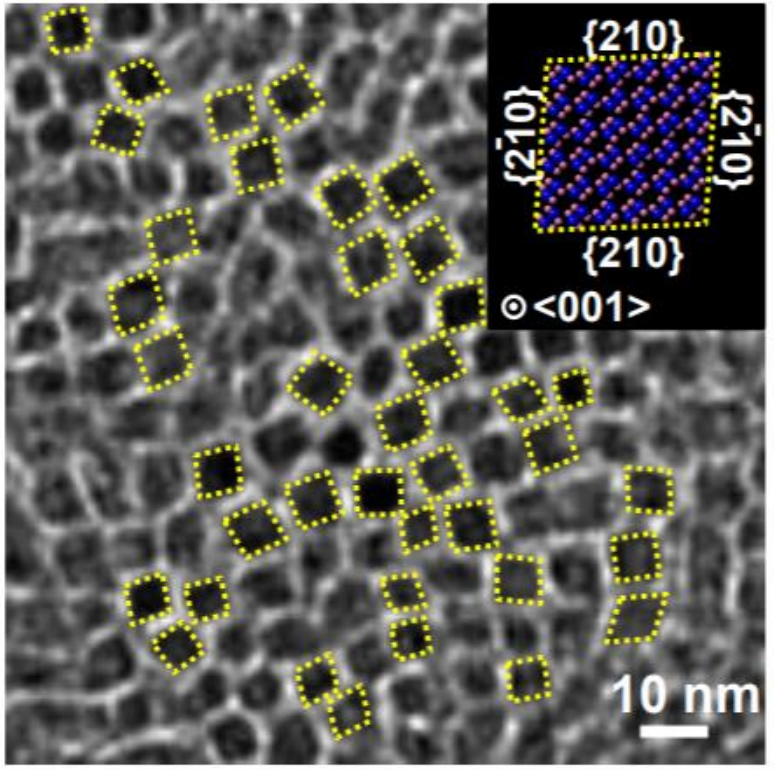
For the first time we know exactly the surface structure Each Co is isolated



Co Catalytic Single-Site in Well-Defined Brookite TiO_2 Nanorod Surface

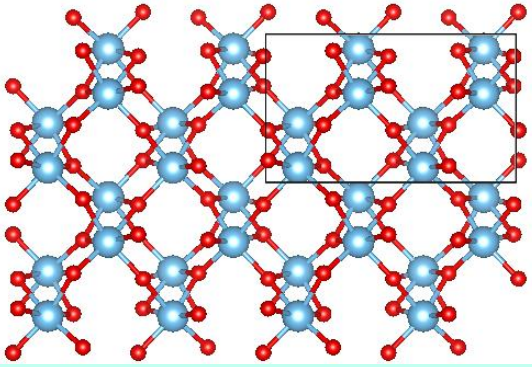
XRD shows brookite single crystal
EXAFS no Co-Co neighbors
Well defined {210} surfaces



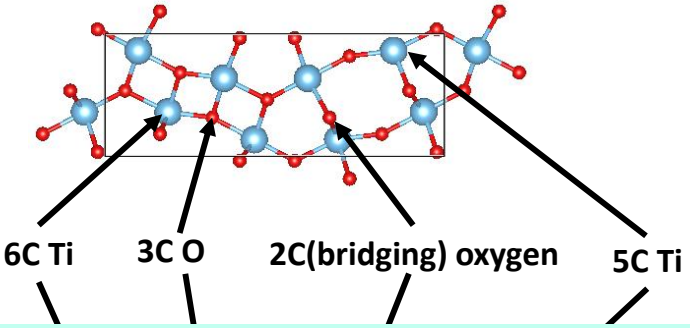


QM calculations on (210) Brookite surface, 12% Co

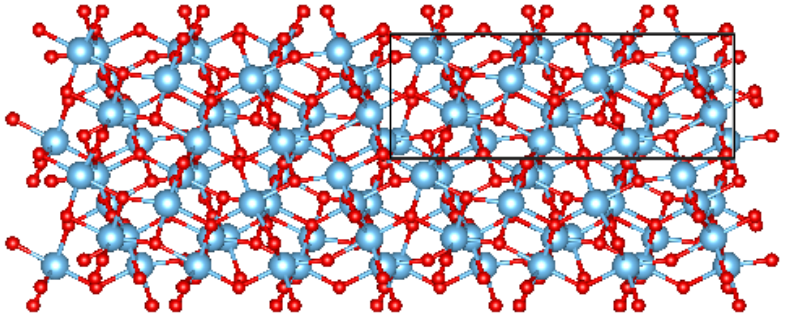
a). Bulk Brookite TiO_2



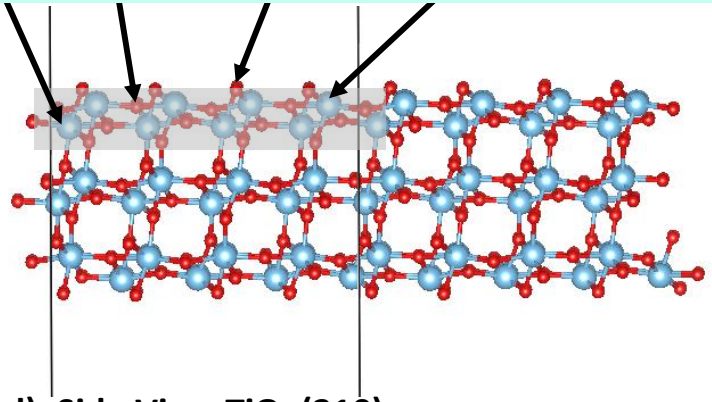
top view of TiO_2(210) surface grey shaded area in d).



There are two types of Ti on this surface: 6 coordinate Ti and 5 coordinate Ti,



c). Top View TiO_2 (210)

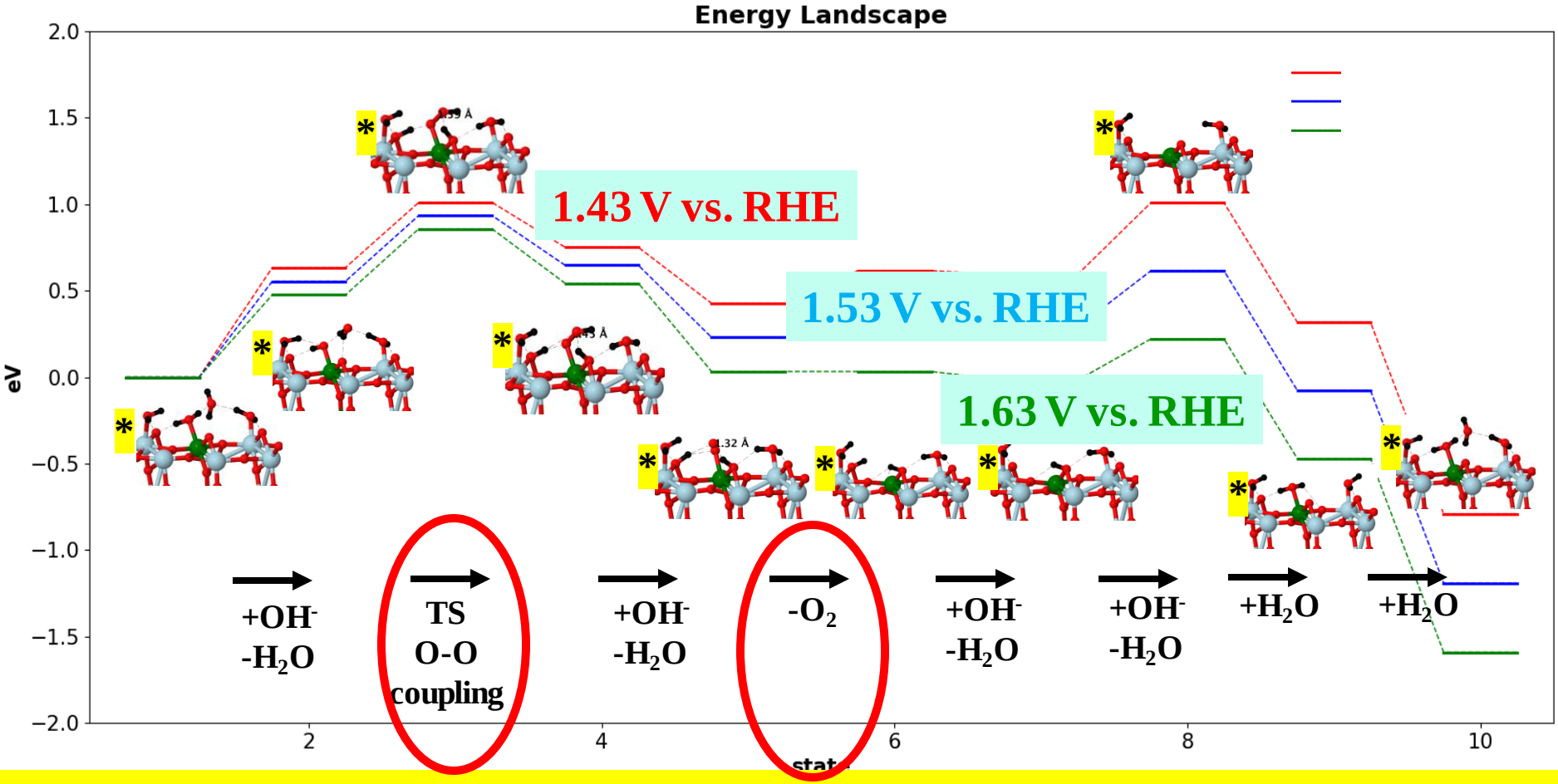


d). Side View TiO_2 (210)

there are two types of O on this surface, 3 coordinate O and bridging O, where 3C O sits lower on z axis, and 2C (bridging) O sits higher on z axis

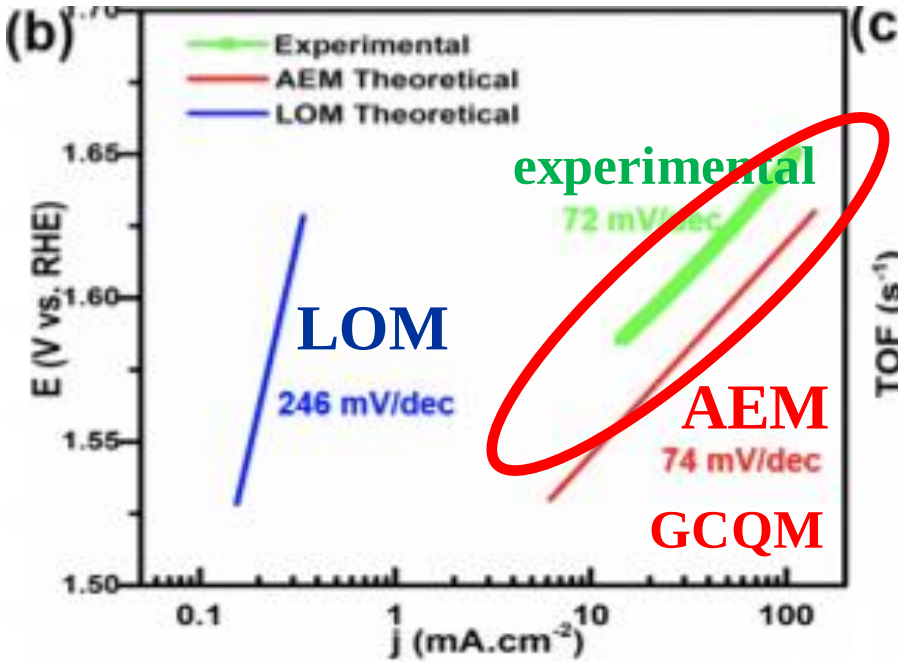
Grand Canonical QM: full QM reaction barriers at constant potential

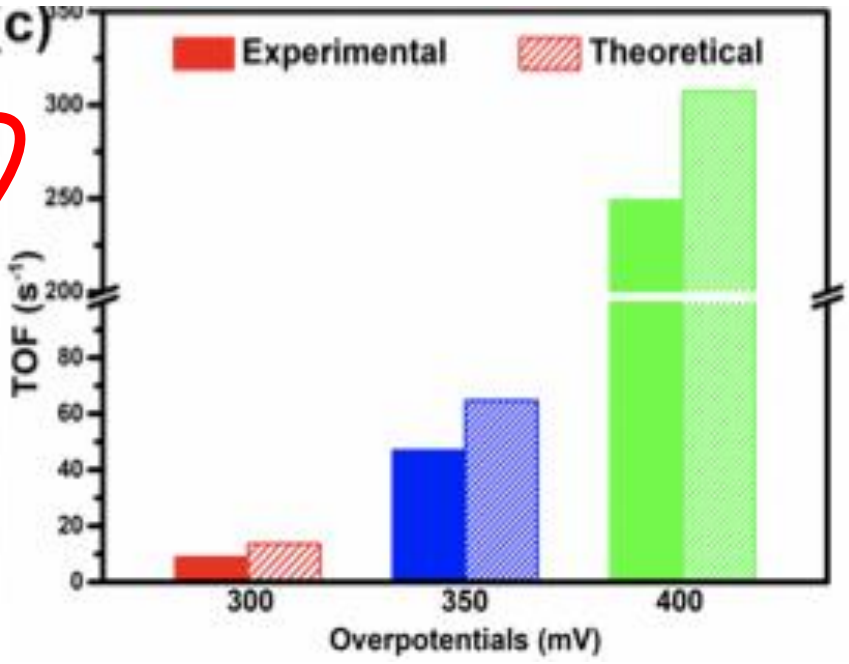
Half Reaction $4OH^- \rightarrow 2H_2O + O_2 + 4e^-$



The OER mechanism involves a M=O bond with radical character on the O atom forming a bond to an OH derived from surface water (referred to as Adsorbate Evolution Mechanism (AEM))

Comparison of GCQM predictions of kinetics with experiment Co-TiO2 SA electrocatalyst





Extremely good comparison for fully characterized surface

GCQM: TOF = 13.1 s^{-1} at η=300 mV per Co SA; TOF = 307.4 s^{-1} at η=400 mV

experiment: TOF = 9.1 s^{-1} at η=300 mV per Co; TOF = 249.2 s^{-1}, at η=400 mV

GCQM: Tafel slope= 74 mV/dec; experimental result of 72 mV/dec

This is the first application of QM based OER kinetics for a system in which the catalyst surface structure is known, validating the very high accuracy for GCQM

Recent breakthroughs

Discover strong anchors between G-Protein and 3 IC loops of GPCR

New mechanism of activation: GP binds first then agonist binding causes activation. Leads to new site for design of agonists

Discover strong anchors between beta arrestin and 3 IC loops of GPCR

Find mechanism of activation for nonbiased ligands

Hope to use in designing biased ligands treat pain and Parkinson's without side effects

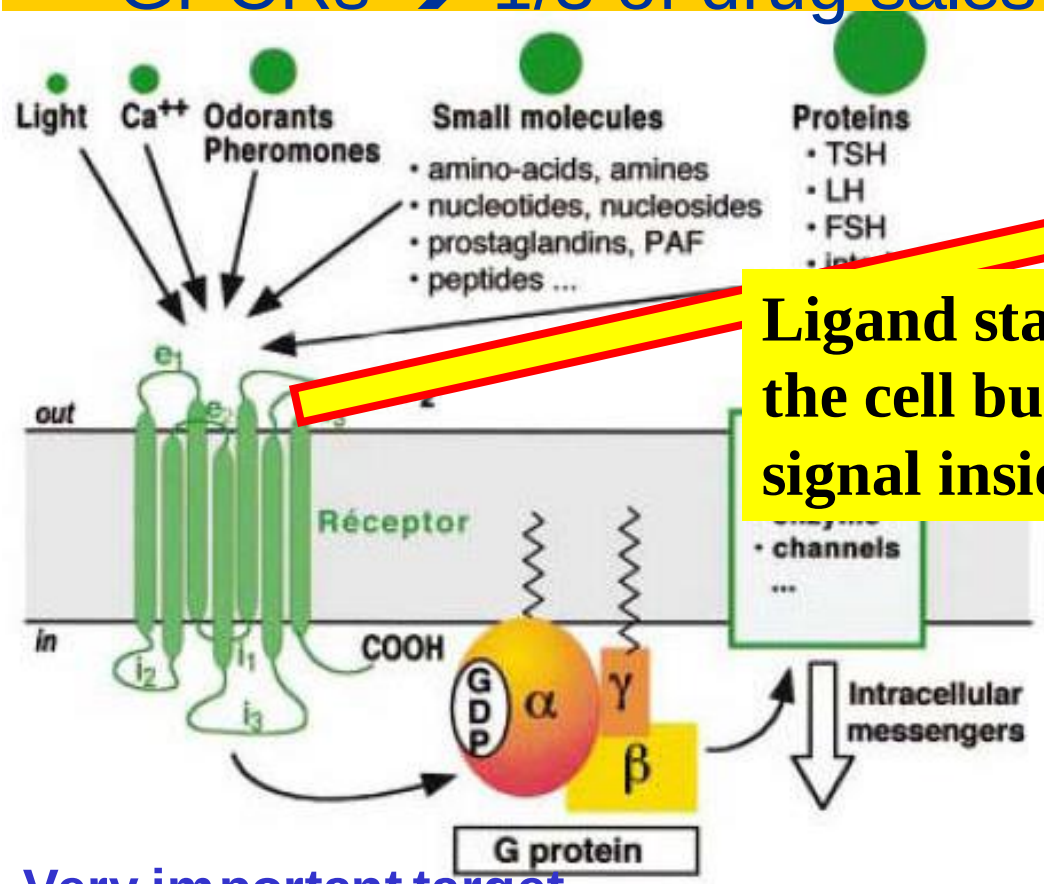
New RexPoN reactive FF, more accurate than DFT. First FF to give correct description of 1st shell. Find Strong HB lifetime 90 fs (new experiment 100 fs). Leads to dynamic 1D polymer network. Explain anomalous properties water at 230K

Developed Machine learning model to predict the activity of the 11,000 surface sites of 10nm nanoparticle. Discover active sites responsible for greatly improved Faraday Efficiency ethanol production.

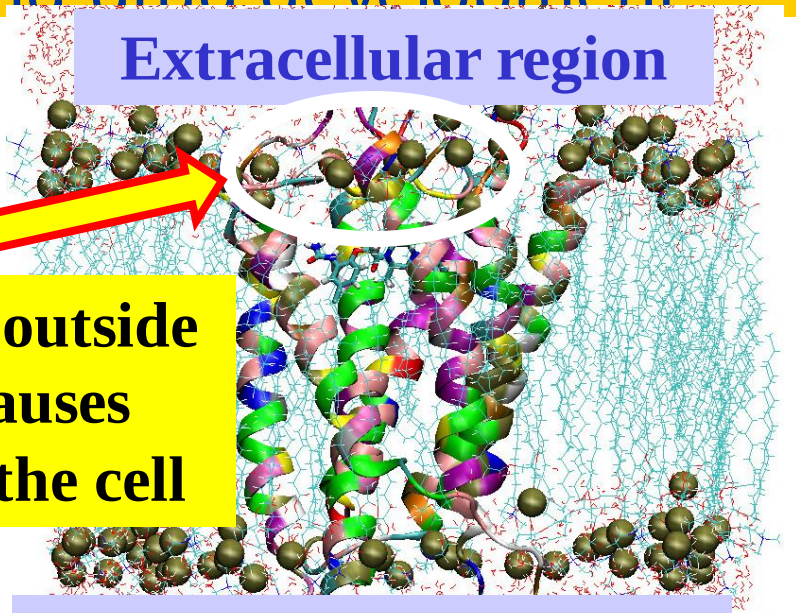
G-Protein Coupled Receptors (GPCRs)

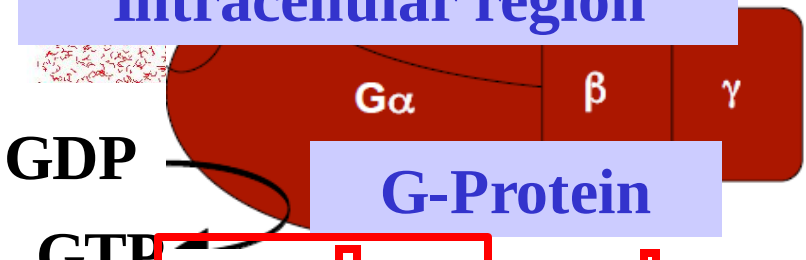
Critical to signaling between cells. 800 human GPCRs

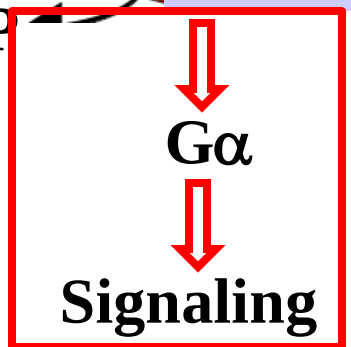
GPCRs ➔ 1/3 of drug sales and drug development



Ligand stays outside the cell but causes signal inside the cell







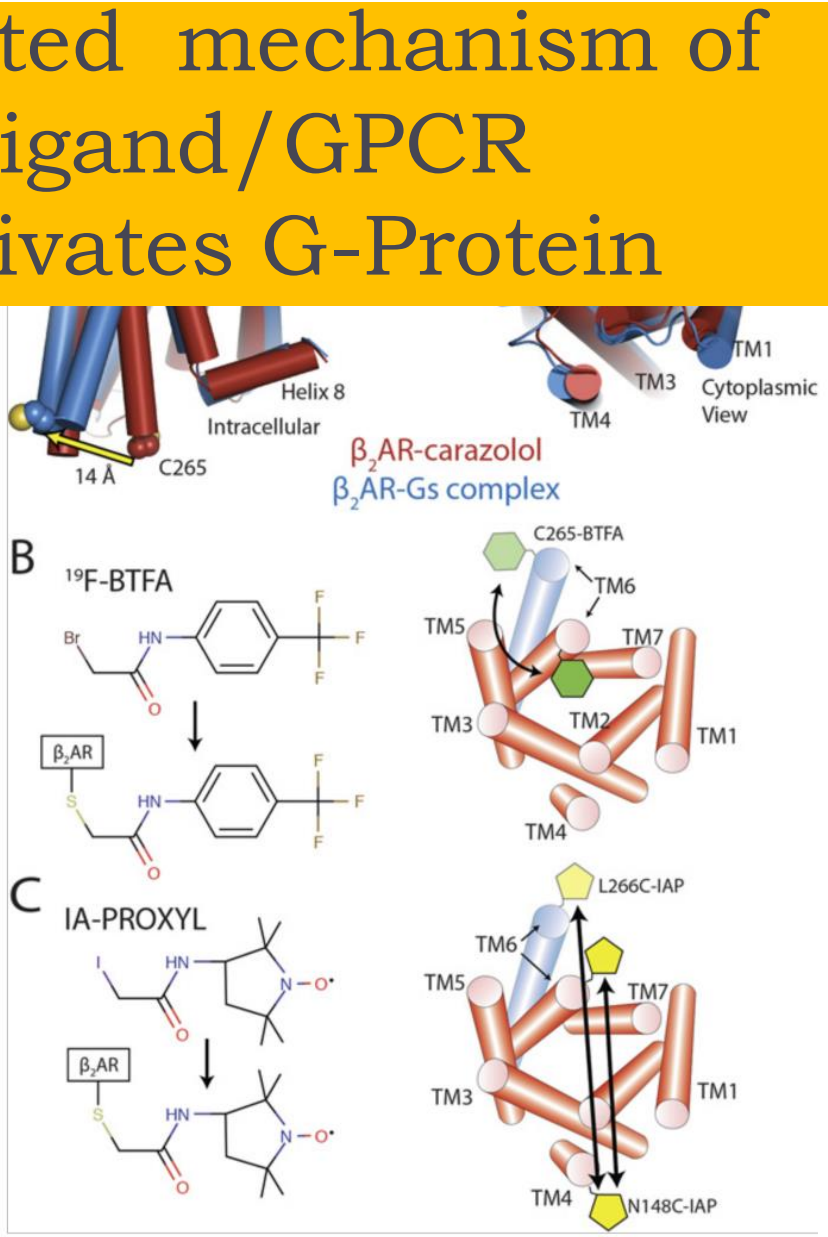
Gβγ

Very important target

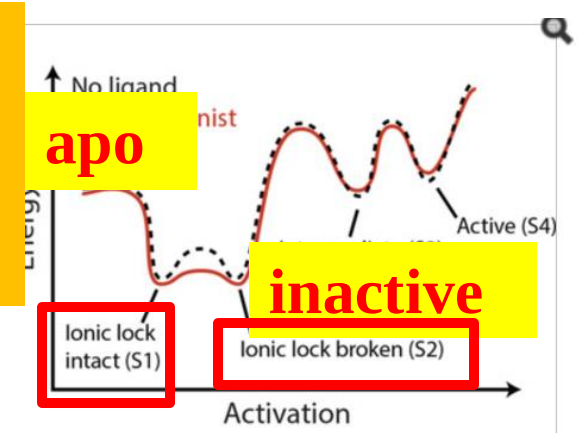
GPCR Sensors (smell, taste, vision, Pain)

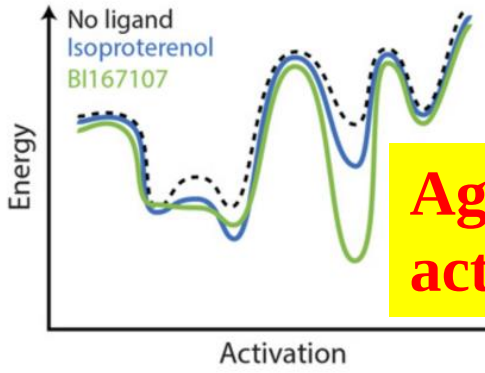
GPCR signaling (acetylcholine, serotonin, bradykinin, adrenoceptors, LPA, S1P1, chemokine Dopamine)

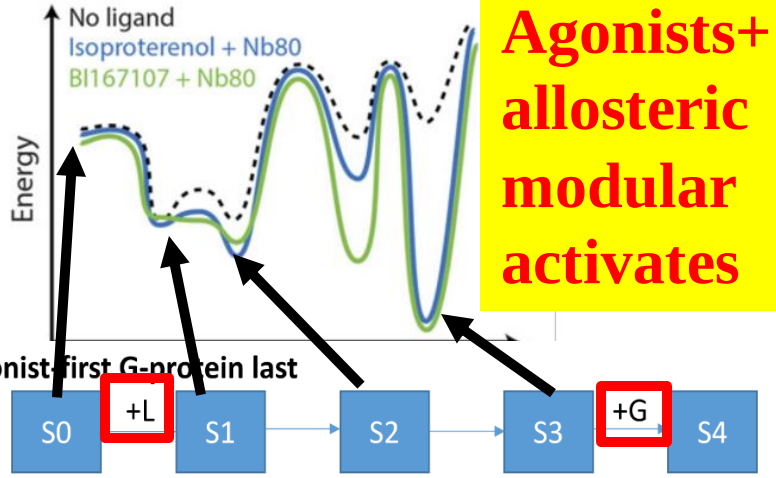
Accepted mechanism of how Ligand/GPCR ➔ activates G-Protein



Spectroscopic methods for detecting conformational changes of β_2AR.

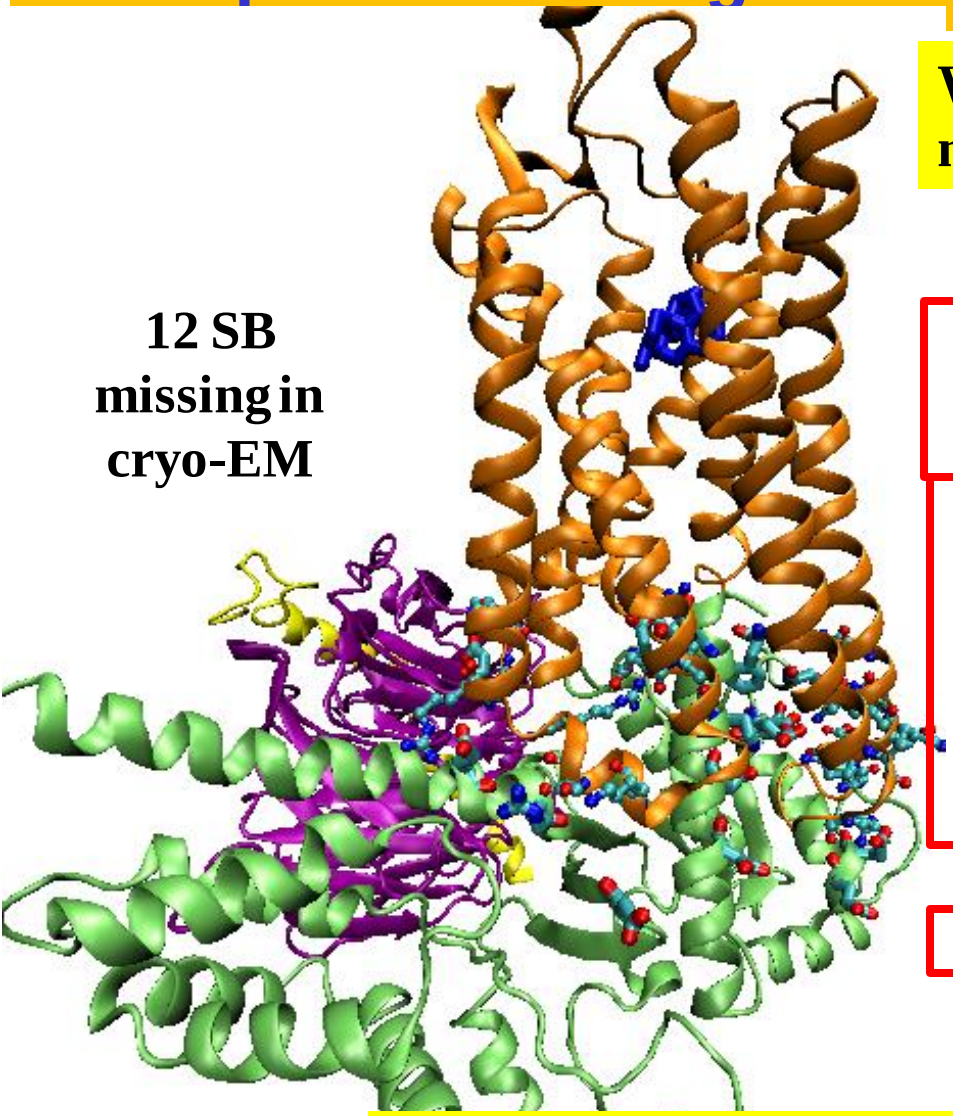






https://www.ncbi.nlm.nih.gov/entrez/eutils/elink.fcgi?dbfrom=pubmed&retmode=ref&cmd=prlinks&id=25981665

Cryo-EM (2018) ➔ structure of full GPCR with Gprotein and agonist – but not resolve SB,HB



12 SB missing in cryo-EM

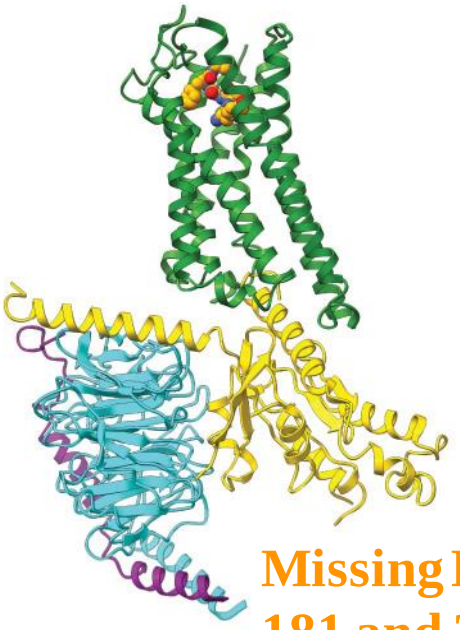
We used SCREAM and metaMD to find the missing SB and HB

Mouse-μOR		Human-μOR	
m-MOR	G-alpha	h-MOR	G-alpha
R179(IL2)	D350	R181(IL2)	D350
R182(4.40)	E28	R184(4.40)	E28
D177(IL2)	R32	D179(IL2)	R32
R263(IL3)	D337	R265(IL3)	E298
D270(IL3)	K314	D272(IL3)	K314
K271(6.26)	D315	K273(6.26)	D315
R277(6.32)	F354(COO-)	R279(6.32)	F354(COO-)
K269(IL3)	E289	K271(IL3)	E289
K271(IL3)	D341	K273(IL3)	D341
m-MOR	G-beta	h-MOR	G-beta
K98(IL1)	D312	K100(IL1)	D312
m-MOR	m-MOR	h-MOR	h-MOR
R179(IL2)	D166(3.49)	R181(IL2)	D166(3.49)

Discovered 3 strong anchors: to ICL1, ICL2, ICL3

Not previously found in xray or cryo-EM

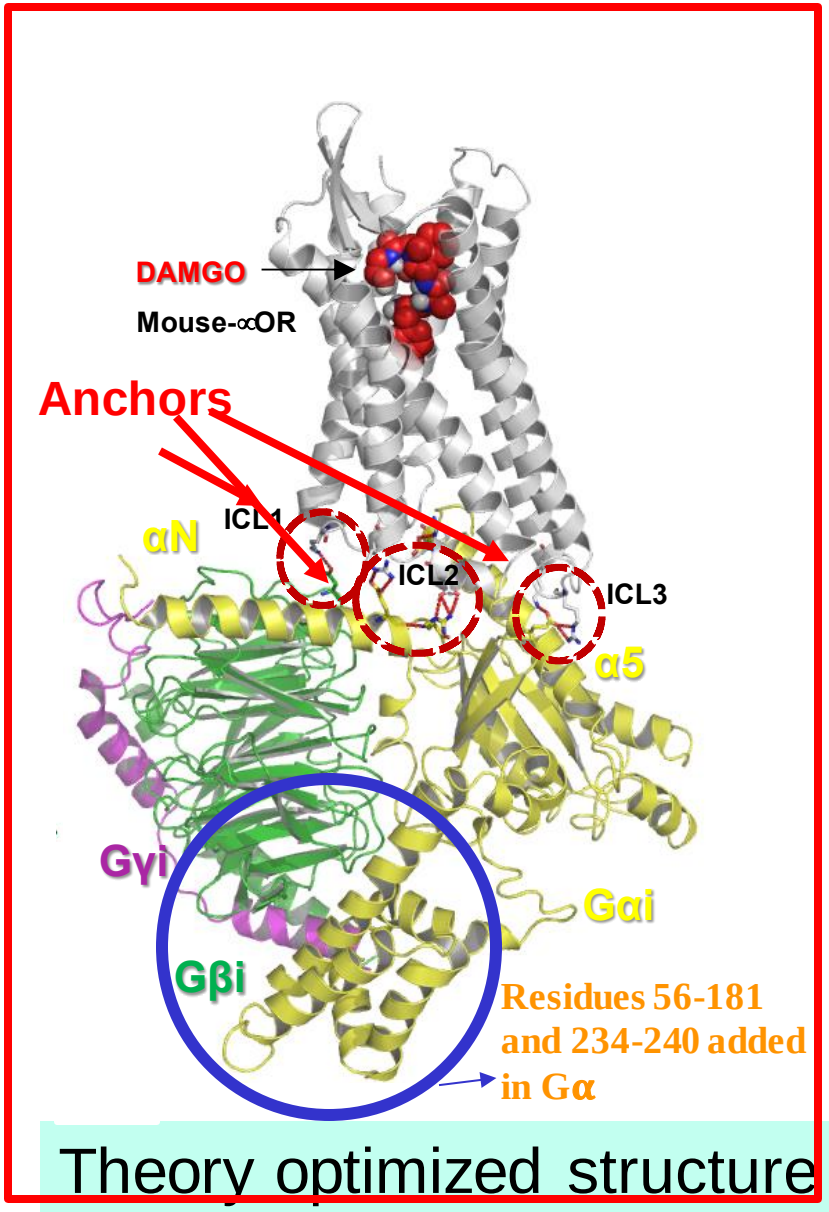
Compare cryo-EM and theory μ-OR-GiProtein



Missing Residues 56-181 and 234-240 in Gα

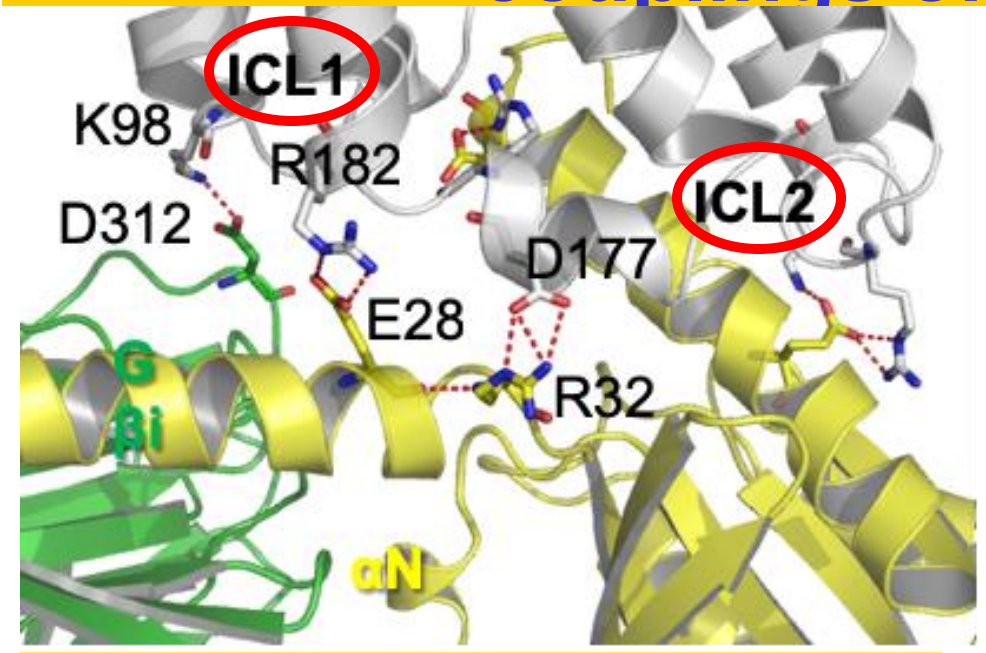
Cryo-EM mouse μ opioid receptor-Gi complex (Resolution 3.2Å)

Keohl et al. ***Nature 2018****, 558, 547*

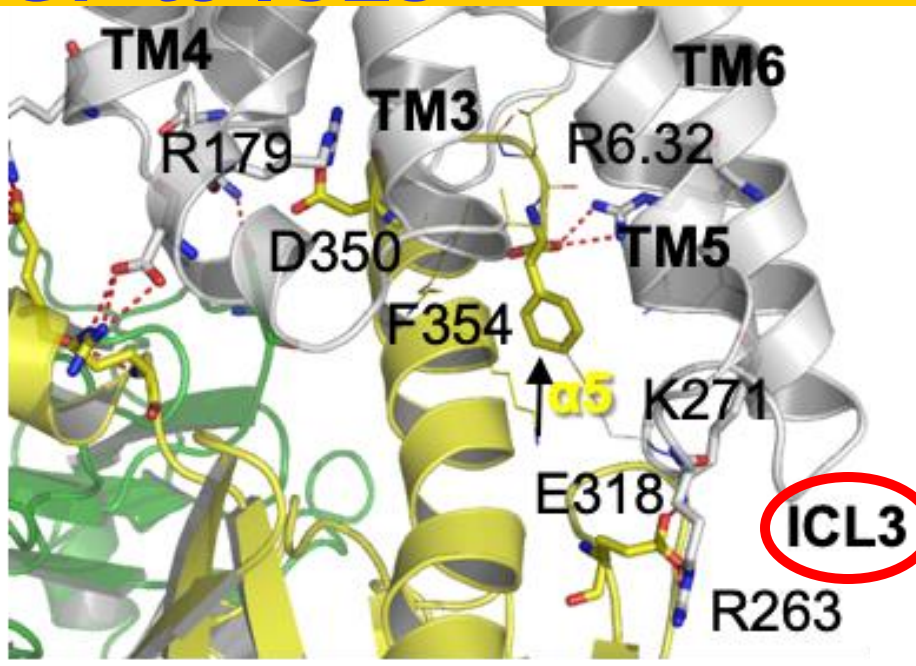


Theory optimized structure

From full structure discovered strong couplings of GP to ICLs



anchors between ICL1 and ICL2 of μOR and GiProtein

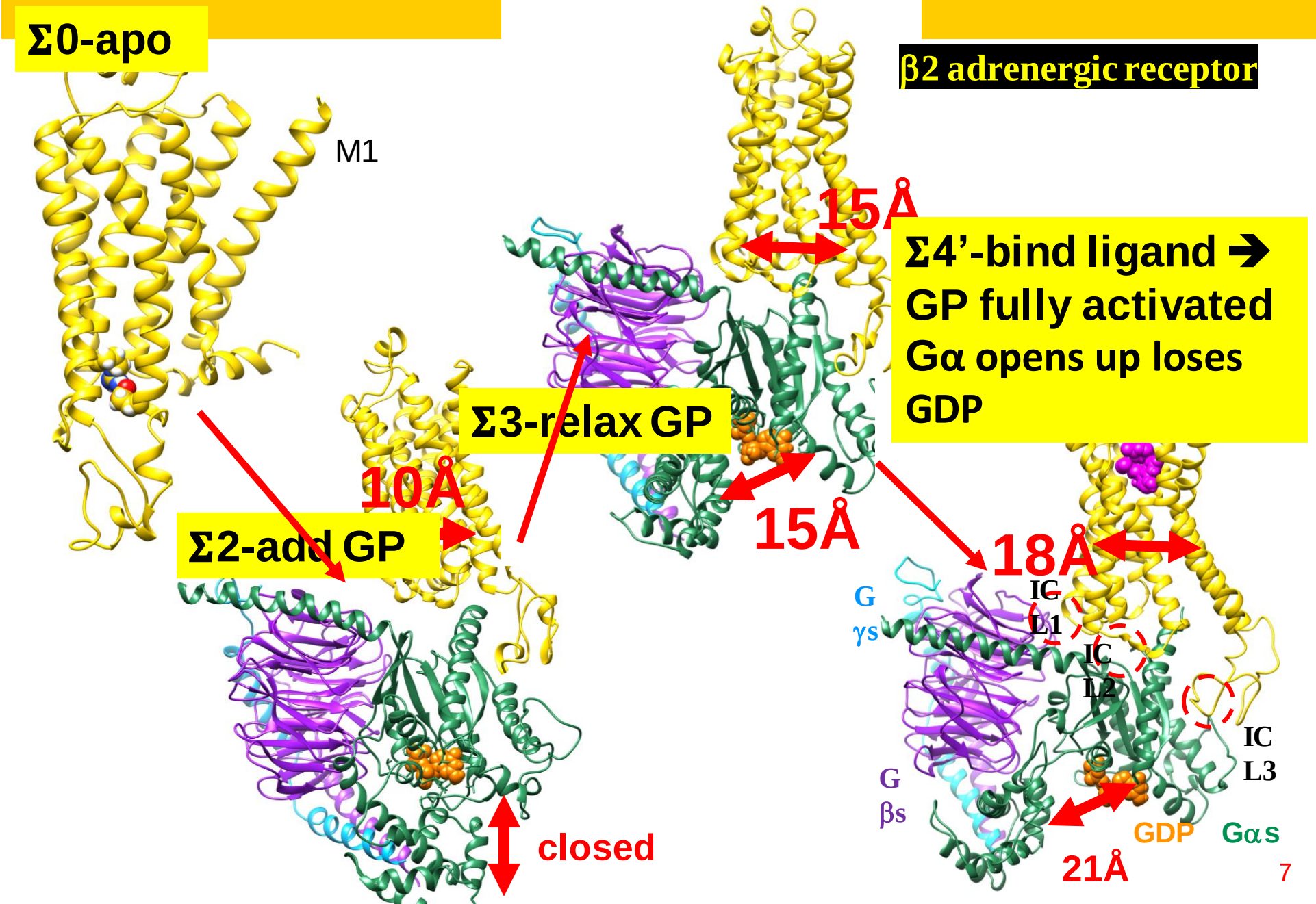


anchors between ICL3 of μOR and GiProtein

The 3 anchors from G-Protein to 3 Intracellular loops of GPCR Lines up the α5 helix just right to insert into GPCR upon agonist activation

Removing agonist ➔ α5 helix retreats back toward GP but 3 anchors still couple strongly ➔ GProtein binds first NOT the agonist

Summarize stages of activation



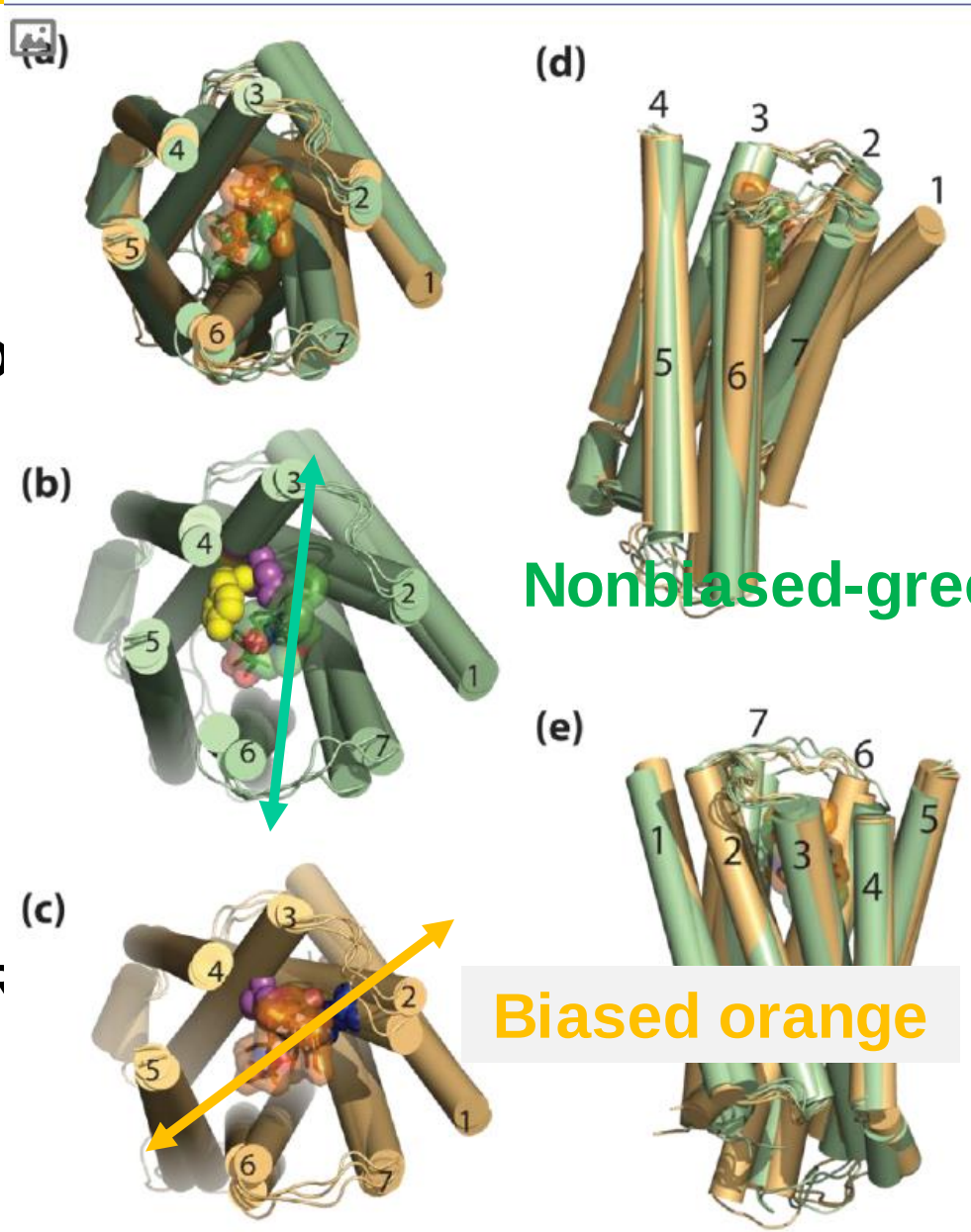
Biased agonists for pain (μ-opioid Receptor)

Morphine is a strong analgesic or painkiller through GProtein signaling from activation of opioid receptors (OR) in the central nervous system.

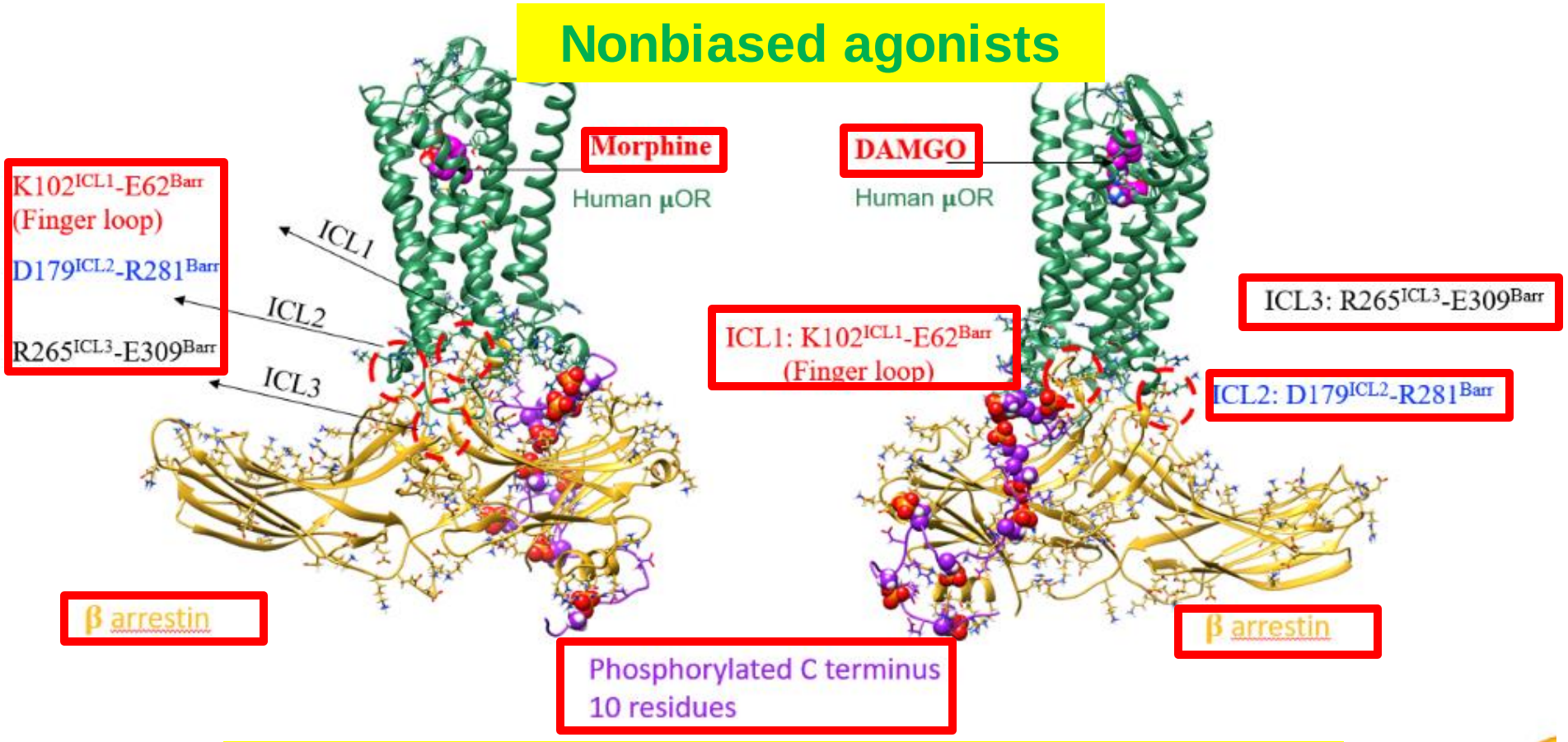
But morphine leads to potentially lethal **side effects mediated by μ-O signaling through the β-arrestin** pathway or by actions at other receptors.

Biased Gi-protein activation with minimal β-arrestin recruitment has been shown alternative efficient and safe pain treatment to replace traditional narcotic analgesics.

There is **strong evidence that μ-OF biased ligands that induce GP signaling but *not* β-arrestin signaling can relieve pain without the side effects**



β-arrestin-GPCR complex μ-Opioid Receptor



Anchors to ICL2 and ICL3 play important roles in stabilizing **β-arrestin-GPCR complex**

New Strategy for very accurate reactive force field

1. **PQEq Charge and Polarization model.** Tested against QM. Predicts QM polarization as point dipoles are brought into various molecules.
2. Determine **long range non-bond parameters** from PBE-D3 or P3LYP-D3 QM that describe Equation of State for molecular solids up to 100 GPa. Extract pure Pauli Principle repulsion (PR) and pure London dispersion (LD) attraction.
3. Given PR and LD, **extract valence parameters to fit exactly highest quality ab initio QM** (CCSDT) for bond breaking and reactions. Describe by ReaxFF formalism
4. Add in **Hydrogen Bonding corrections** from QM on dimers at CCSDT. 30,000 points fitted to analytic functions to ~ 4 cm-1 (Joel Bowman, Emory)

S. Naserifar & W.A. Goddard III. The quantum mechanics-based polarizable force field for water simulations. J. Chem. Phys. **149** (17):174502 (2018) DOI: 10.1063/1.5042658

Properties of water

Empirical FF | DFT-QM based FF

	Expt.	RexPoN	TIP3P	TIP4P-2005	SPC/E	PBE	SCAN	MB-pol	CC-pol
T_{melt}	273.15	273.3	146	252	215	420	-	263.5	-
S^0	69.9	68.43	72.51	57.47	60.30	51.32	-	-	-
ρ	0.9965	0.9965	0.98	0.993	0.994	0.944	1.050	1.007	-
ε	78.4	76.1	94	58	68	112	-	68.4	-
ΔH_v	10.52	10.36	10.05	11.99	11.79	6.20	-	10.93	10.89
R_1	2.86	2.84	2.79	2.77	2.75	2.71	2.74	2.81	2.79
g_{OO} (R_1)	2.50	2.34	2.79	3.22	3.05	3.69	3.17	2.76	2.77

nelting temperature T_{melt} (K) at 1 atm pressure.
tandard molar entropy S^0 (J/mol/K)[27],
ensity ρ (g/cm^3),
tatic dielectric constant ε,
eat of vaporization ΔH_v (kcal/mol),
$_1$ (Å) the position of the first peak of g_{OO}
ll at T= 298 K, p=1 atm.

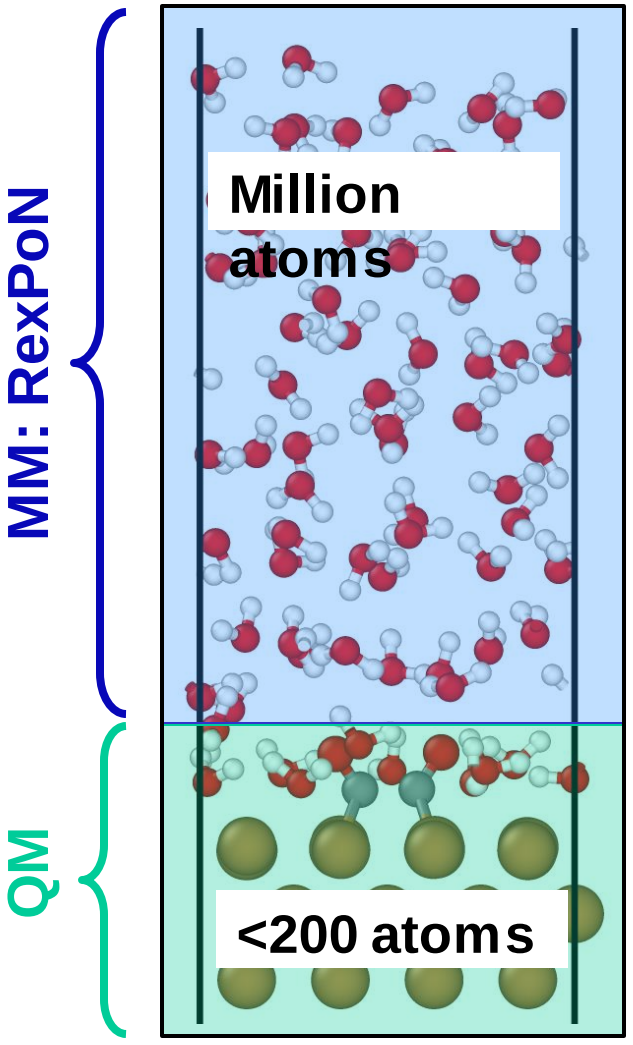
RexPoN make NO use of empirical data
Only high level QM
But it leads to spectacular agreement with experiment

kip the details, jump to the summary

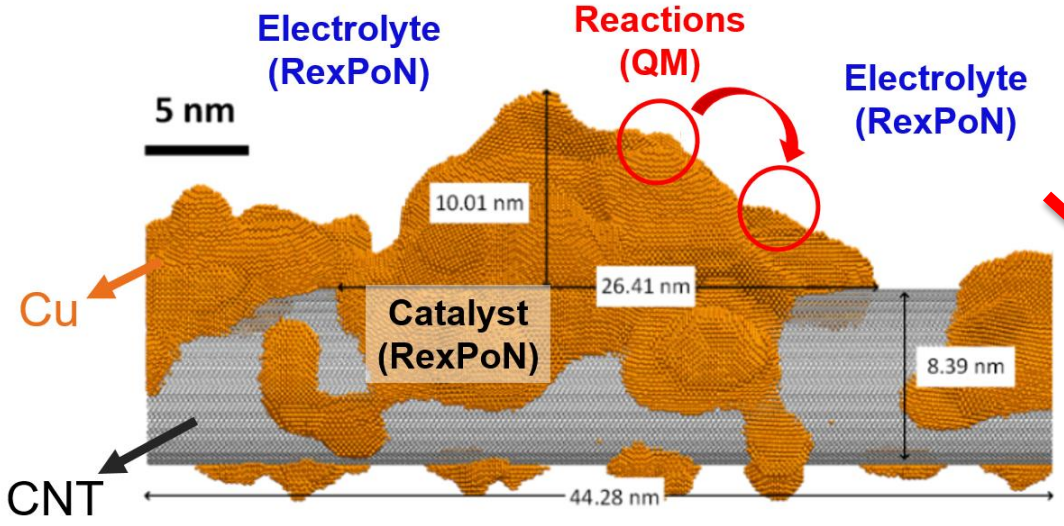
RexPoN Embedded QM (REQM)

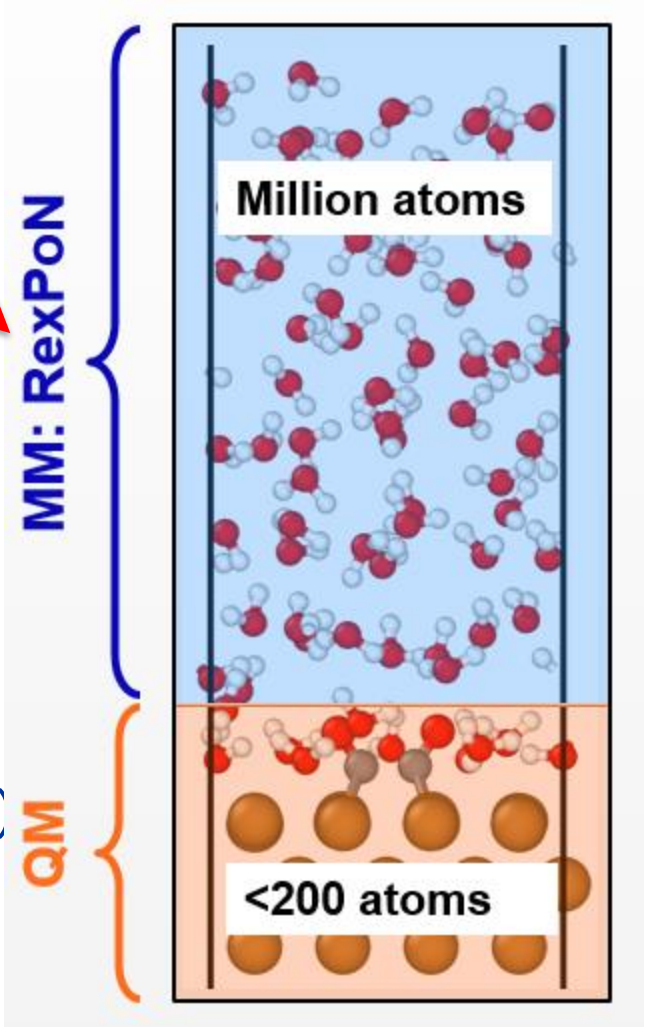
- QM/MM: a great idea (Noble prize in 2013) but many challenges!
- Explicit coupling is often needed; cannot include polarization effects of MM in the QM region.

- RexPoN accurately describes the long-range polarization effects (of full solvent) in QM region.
- RexPoN accurately describes the long-range van der Waal attraction from QM
- In addition, RexPoN bond breaking curve fits QM (CCS) exactly. no discontinuity in forces



RexPoN embedded Quantum Mechanics (REQM) describe full millions atoms with RexPoN QM based reactive FF
Select 200 atom region for QM, focus QM on reactions at the interface. Move QM region to examine different spots

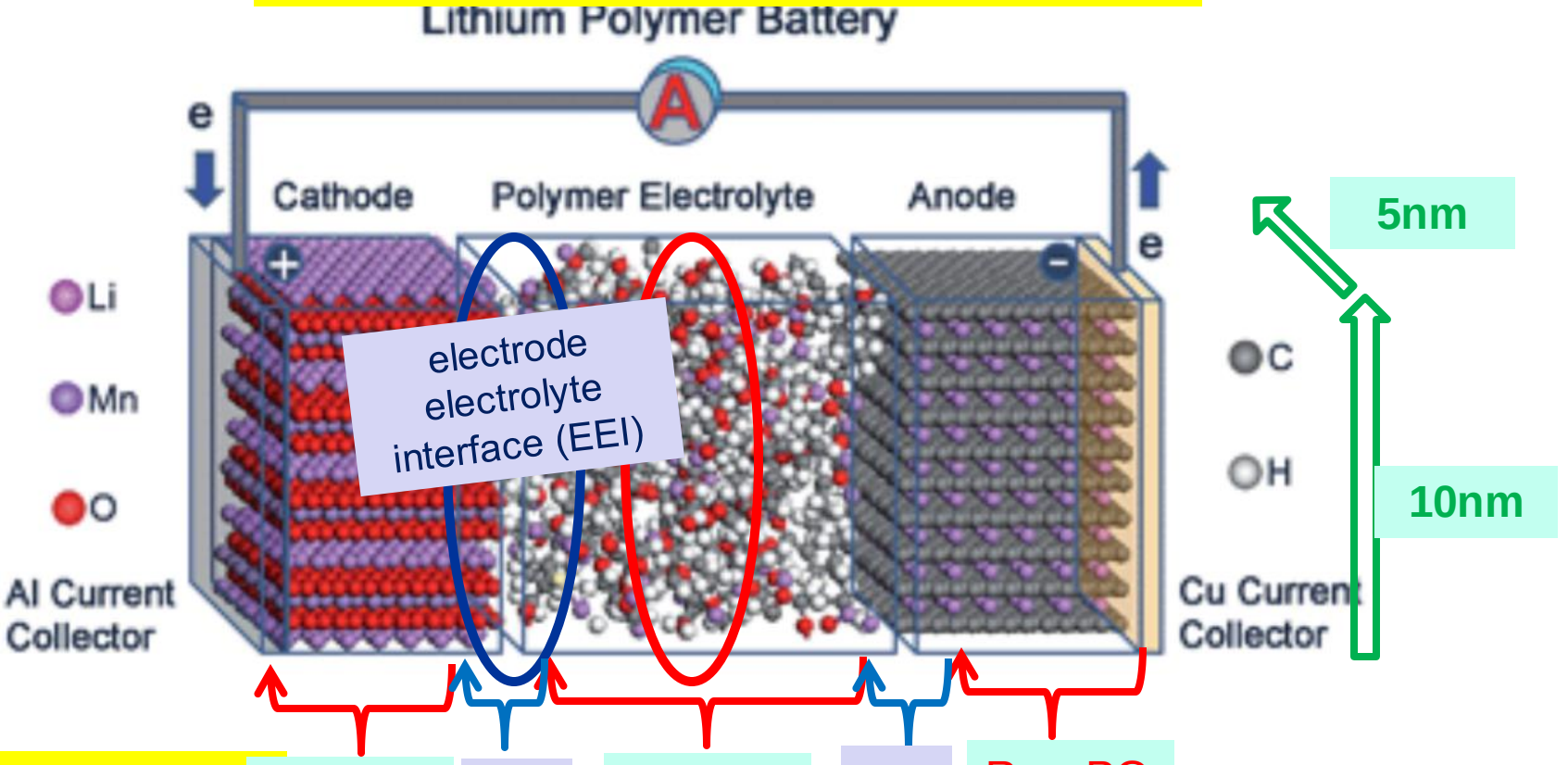




Periodic box 44nm x 22 nm x 22 nm (7 million atoms)
Carbon support (here carbon nanotube)
Catalysts deposit (200,000) atoms
Solvent: H2O, pH=1, positive and negative atoms

Application new generations batteries fuel cells: predict chemistry & charge flow at electrode electrolyte interface (EEI) WHILE describing diffusion, ions etc throughout the device

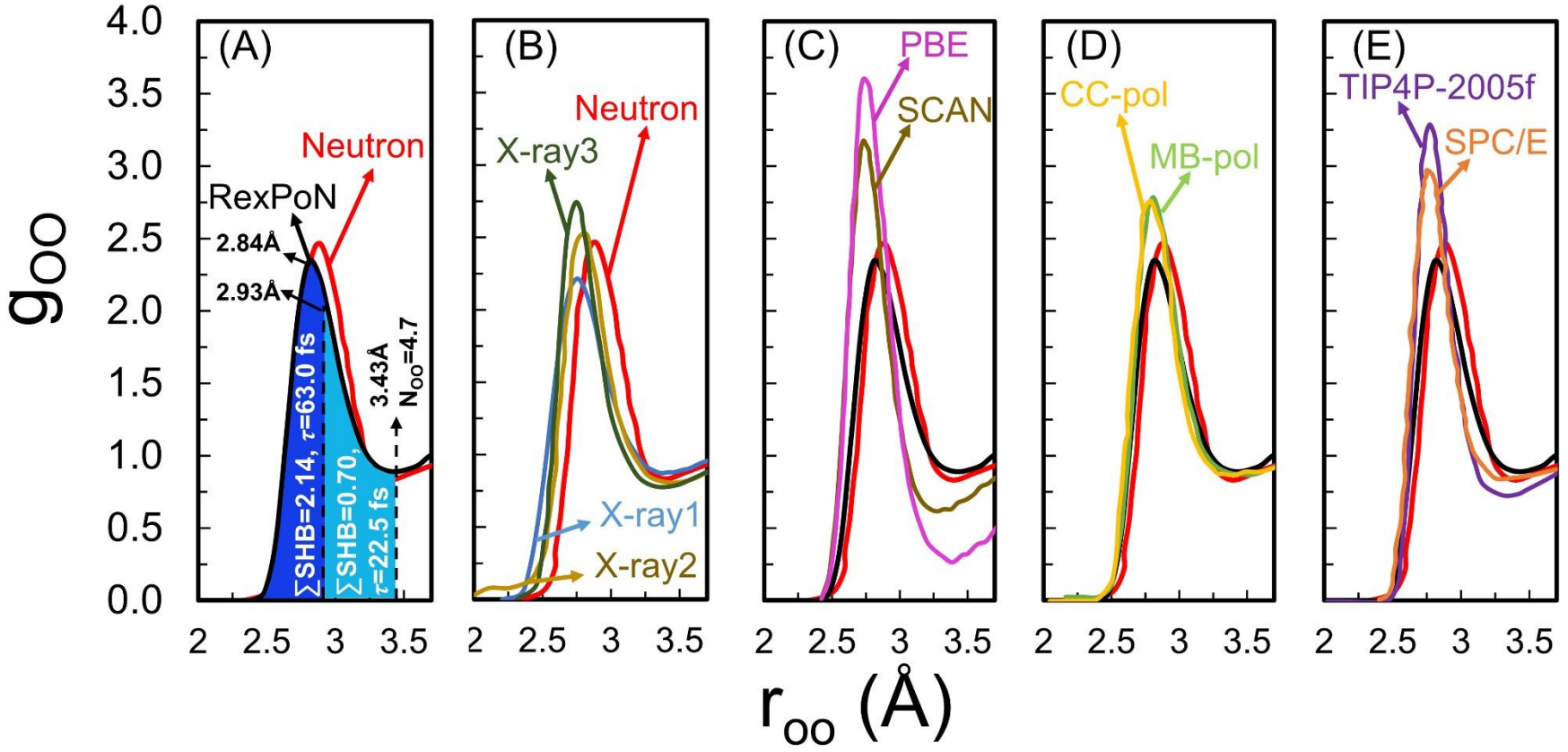
Target: QM/RaxPoN on full device



10 ps QM metadynamics
Each point 1ns
RexPoN

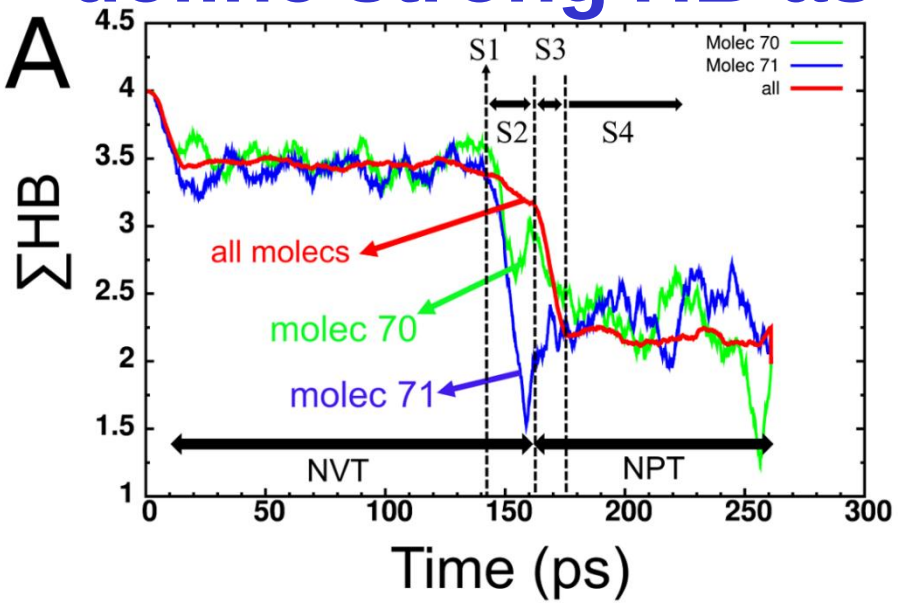
1.2 million atoms
RexPoN
300 atoms QM

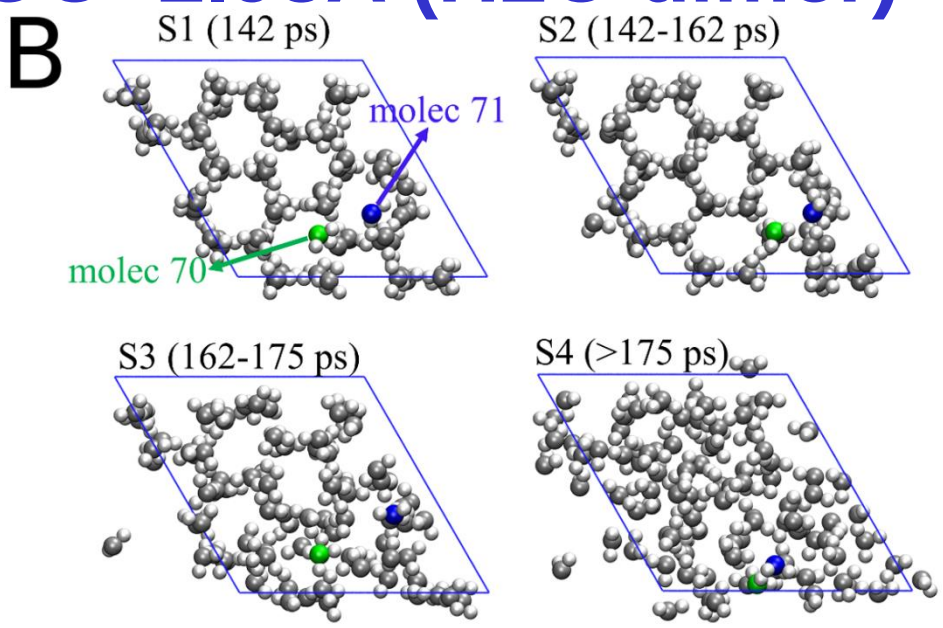
OO radial distribution
Only direct experimental property related to structure



Only RexPoN captures the OO radial distribution
Even DFT QM (PBE and SCAN do NOT get it

Initial steps of melting at 273.5K
define strong HB as OO<2.93A (H2O dimer)





Water heated 0 K to 273.5 K over 10 ps followed by MD-*NVT* for 150 ps.
Volume allowed to adjust to 1 atm during 100 ps of MD-*NPT* simulations.

Initiation melting dominated by blue and green waters in same hexagonal ring of ice at 142 ps adjacent blue and green molecules start to break out of its hexagonal ring, sum SHB drops from 3.5 to 2.7 at 153 ps.

The **sum SHB of blue goes down to 1.5 at 158 ps Green goes back to 3 at 162ps**
162 to 175 ps the blue and green molecules in, out of the hexagonal rings repeatedly
whole structure melts at 175ps ➔ sum SHB=2.18

Ice has 4 strong HBs, just after melting,water has only 2.2 strong HBs

Now we have the most accurate ever QM based description of water

Define Strong HB as R=2.93 (H2O dimer)
sum of SHB on any H2O = 4.0 for ice
we find a sharp drop from sum SHB=4.0 for 273 K to 2.28 at 273K, which decreases to sum SHB=2.14 at 298K and 1.85 at 350K.
We were shocked by these unexpected results.

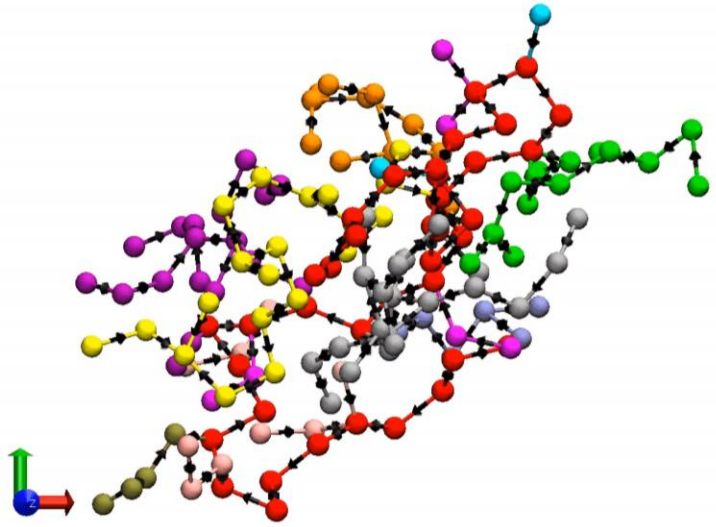
T (K)0	M_c	∑HB	SD	SHB lifetime (fs)	Density (gr/cm3)
150	216 (∞)	3.14	1.55	175	-
273.5	177 (∞)	2.28	1.08	101	-
277	168 (∞)	2.22	1.05	103	1.000
298	148 (∞)	2.14	1.00	90	0.9965
350	72	1.85	0.84	78	0.960
400	36	1.63	0.71	68	-

SHB lifetime

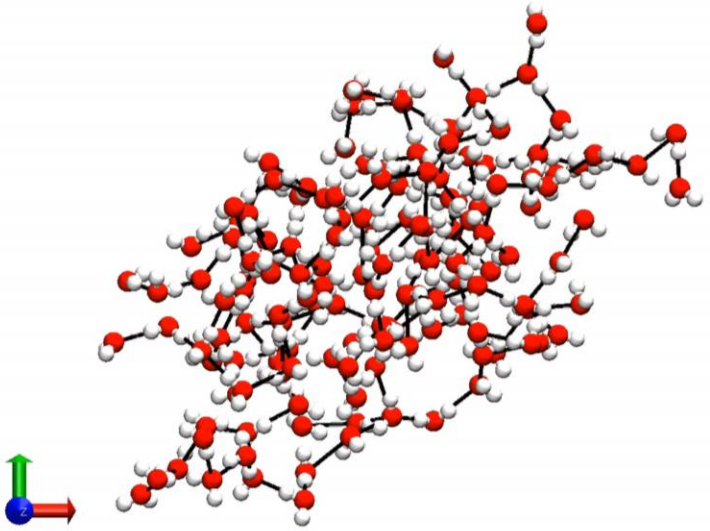
Liquid water at 298K has ~2 Strong HB, with lifetime ~90 femtoseconds

Liquid Water is a Polymer

- The SHBs connect to form a **dynamic high molecular weight branched polymer**.
- Average number of strong HB at 298K ≈ 2.0. That is a 1 dimensional chain structure.



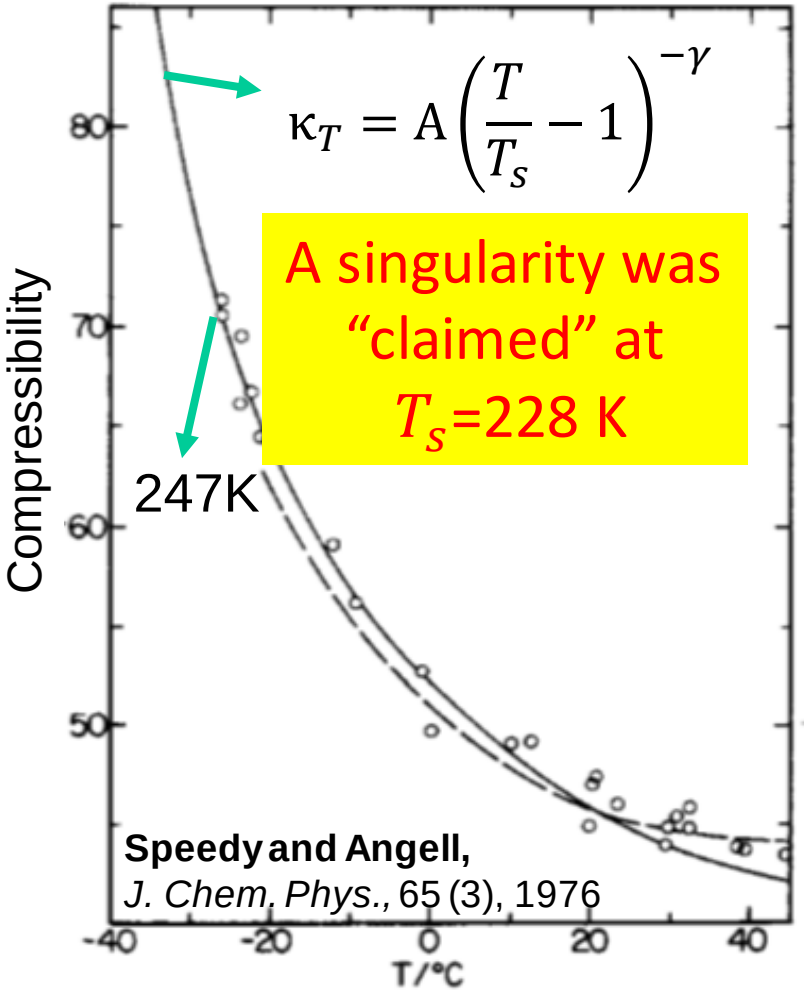
(A) The polymer backbone (longest chain) is shown in red.



(B) Same structure as in (A) but showing the OH bonds.

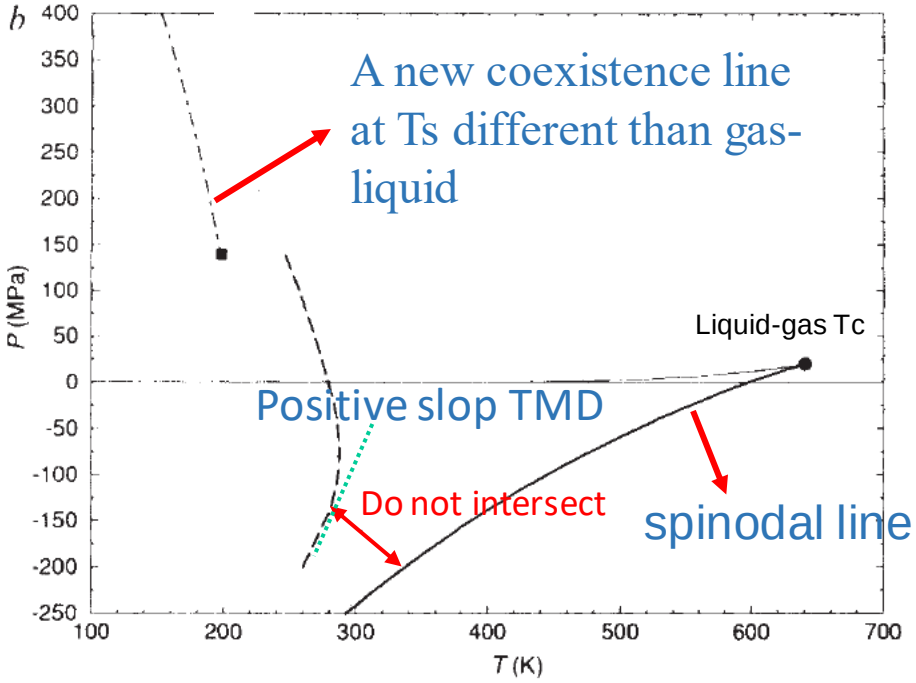
S. Naserifar & W.A. Goddard III. Liquid water is a dynamic polydisperse branched polymer. Proc. Natl. Acad. Sci. U.S.A. **116** (6):1998-2003 (2019) DOI: 10.1073/pnas.1817383116

Anomalies of Deeply Supercooled Liquid Water
Liquid-Liquid Critical Point (LLCP) Hypothesis -1992



2 Phases Liquid

ST2 Model Simulations

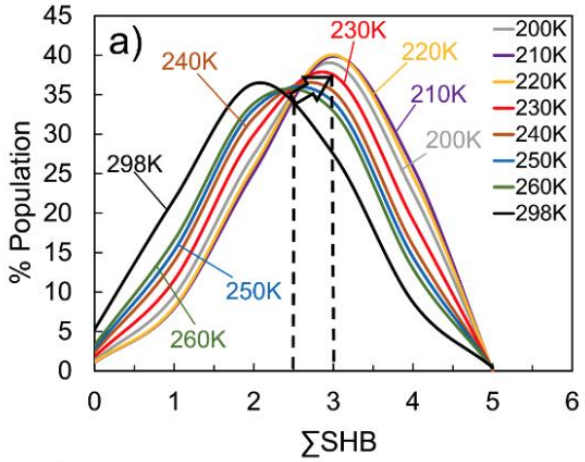


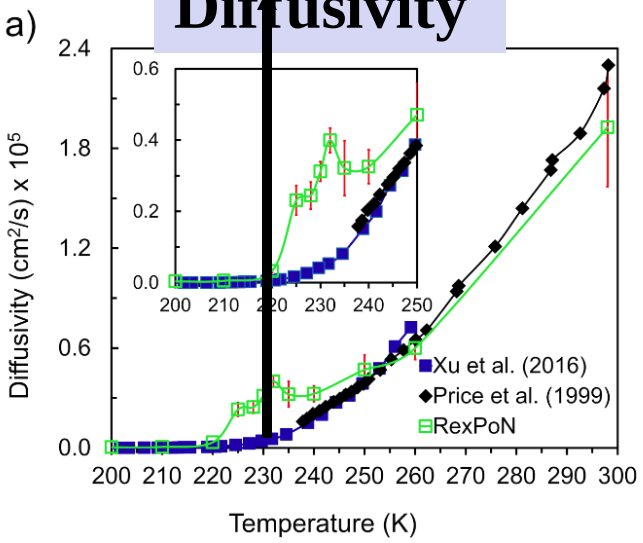
- Non-continuous spinodal line with positive slope.
- Coexistence of high and low density liquids at Ts.

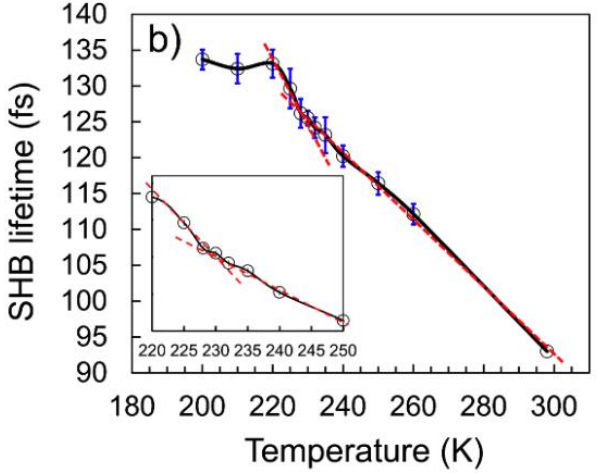
1 at

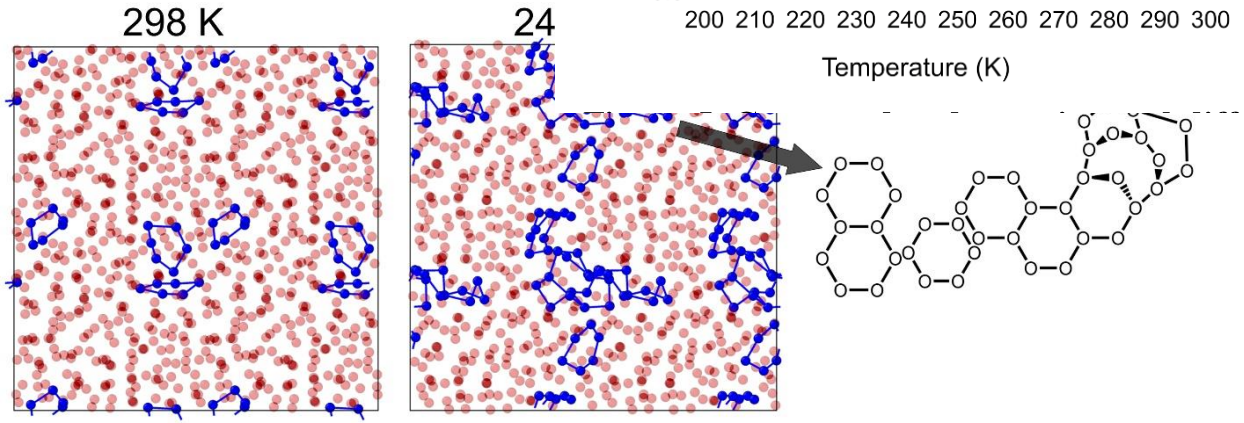
Stanley et al , *Nature* 360, 6402 (1992)

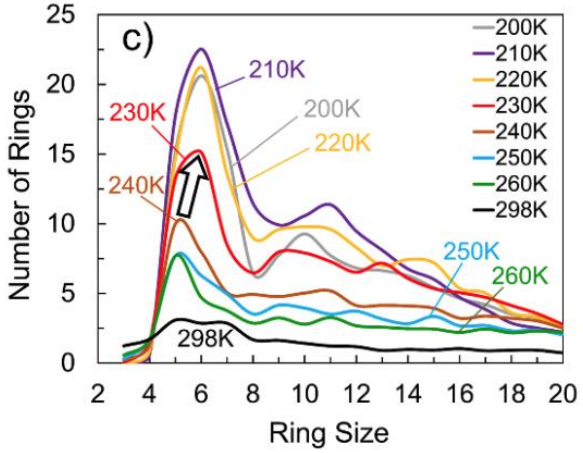
Diffusivity

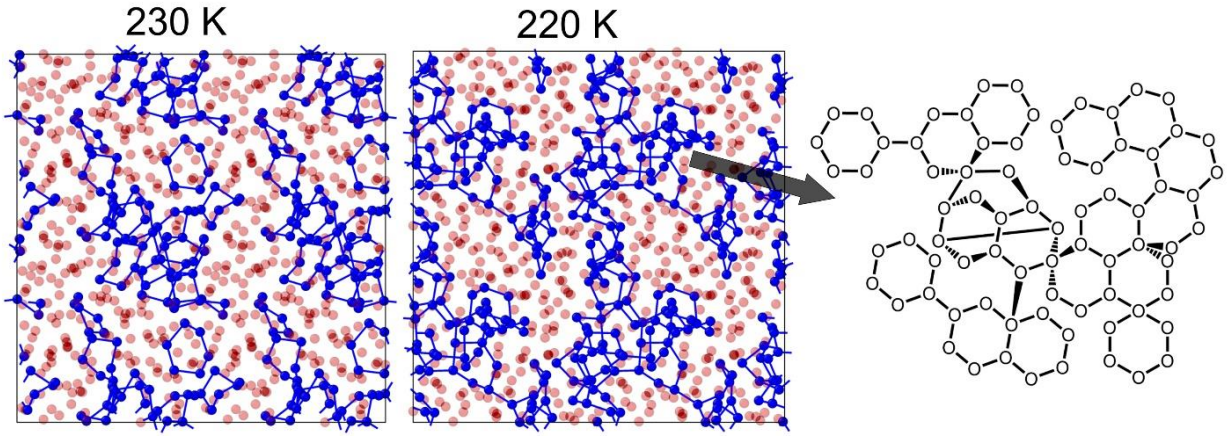




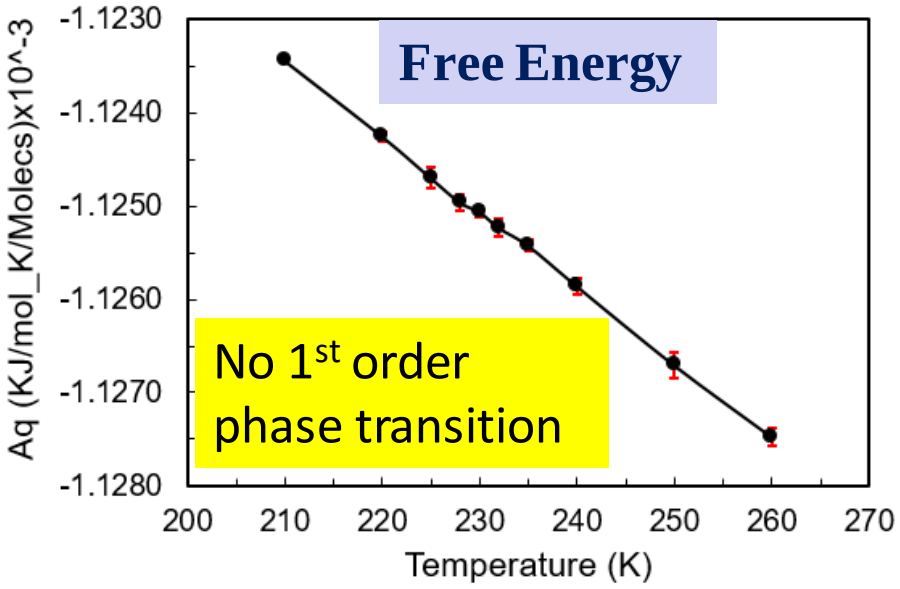


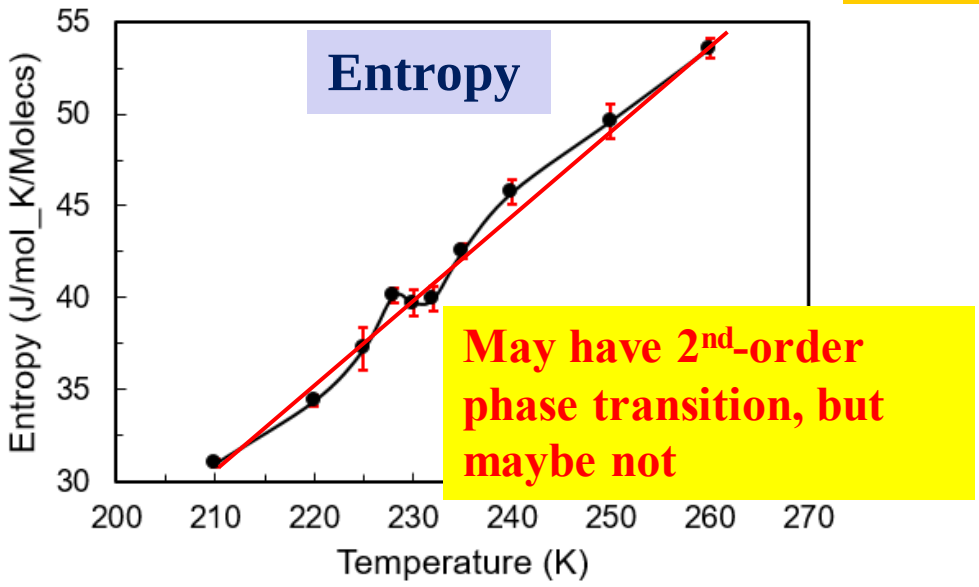






Free Energy, Entropy, Diffusivity of H2O (using 2PT Method)





- Therefore, only one phase at each temperature.
- No Liq-Liq Crit point
- No phase transition.
- Instead have a topology transition, which leads to dramatic change in dynamical properties

Experimental-Theory collaborations over the years in CCE

Alison Ondrus
Linda Hsieh-Wilson
Theo Agapie

current

Harry Gray
Jim Heath
Greg Fu
David Tirrell
Frances Arnold
Dennis Dougherty
Bob Grubbs
Sossina Haile
Rick Flagen
Nate Lewis
Jack Beauchamp
Ahmed Zewail
Costas Giapis
John Seinfeld
Brian Stoltz
Judy Campbell

Also
Harry Atwater
Bill Johnson
Paul Asimov
Mike Hoffmann

current

First principles theory and simulation are now at the point where it can drive the design and development of new materials

- Artificial photosynthesis
- Photo CO2 reduction
- Fuel Cell,
- Battery,
- Solar cells
- Water Purification,
- CO2 Sequestration
- Energy
- Hydrogen