

ESTEBAN VOHRINGER-MARTINEZ

DOCTOR GEORG-AUGUST-UNIVERSITÄT GÖTTINGEN, ALEMANIA, 2008

LÍNEA(S) DE INVESTIGACIÓN O ÁREAS DE TRABAJO

✓ QUÍMICA TEÓRICA, CATÁLISIS ENZIMÁTICA

LISTADO DE PUBLICACIONES EN LOS ÚLTIMOS 10 AÑOS

Vöhringer-Martinez, E; Hansmann, B; Hernandez-Soto, H; Hernandez, H; Francisco, J S; Troe, J; Abel, B. **2007**. *Water catalysis of a radical-molecule gas-phase reaction*. **Science**:**5811 315:497-501**.

Link, Oliver; Vöhringer-Martinez, Esteban; Lugovoj, Eugen; Liu, Yaxing; Siefermann, Katrin; Faubel, Manfred; Grubmüller, Helmut; Gerber, R Benny; Miller, Yifat; Abel, Bernd. , **2009**. *Ultrafast phase transitions in metastable water near liquid interfaces*. **Faraday discussions**: **141:67-79; 81-98**.

Haas, Jürgen; Vöhringer-Martinez*, Esteban; Bögehold, Andreas; Matthes, Dirk; Hensen, Ulf; Pelah, Avishay; Abel, Bernd; Grubmüller, Helmut. **2009**. *Primary steps of pH-dependent insulin aggregation kinetics are governed by conformational flexibility*. **Chembiochem : a European journal of chemical biology** **11 10:1816-22**.

Vöhringer-Martinez, E; Tellbach, E; Liessmann, M; Abel, B. **2010**. *Role of water complexes in the reaction of propionaldehyde with OH radicals*. **The Journal of Physical Chemistry. A**:**36 114:9720-4**.

Vöhringer-Martinez, Esteban; Toro-Labbé, Alejandro. **2010**. *The role of water in the proton transfer reaction mechanism in tryptophan*. **Journal of Computational Chemistry**:**14 31:2642-9**.

Vöhringer-Martinez, Esteban; Toro-Labbé, Alejandro. **2010**. *Amino acids at water-vapor interfaces: surface activity and orientational ordering*. **The Journal of Physical Chemistry. B**:**40 114:13005-10**.

Hargis, Jacqueline C; Vöhringer-Martinez, Esteban; Woodcock, H Lee; Toro-Labbé, Alejandro; Schaefer, Henry F. **2011**. *Characterizing the mechanism of the double proton transfer in the formamide dimer*. **The Journal of Physical Chemistry. A**:**12 115:2650-7**.

Duarte, Fernanda; Vöhringer-Martinez, Esteban; Toro-Labbé, Alejandro. **2011**. *Insights on the mechanism of proton transfer reactions in amino acids*. **Physical chemistry chemical physics : PCCP**:**17 13:7773-82**.

Vöhringer-Martinez, Esteban; Toro-Labbé, Alejandro. **2011**. *The mean reaction force: a method to study the influence of the environment on reaction mechanisms*. **The Journal of Chemical Physics: 6 135:064505**.

Liu, Yuli; Burger, Steven K; Ayers, Paul W; Vöhringer-Martinez, Esteban. **2011**. *Computational study of the binding modes of caffeine to the adenosine A2A receptor*. **The Journal of Physical Chemistry. B:47 115:13880-90**.

Vöhringer-Martinez, Esteban; Toro-Labbé, Alejandro, **2012**. *Understanding the Physics and Chemistry of Reaction Mechanism from Atomic Contributions: A Reaction Force Perspective*, **Journal of Physical Chemistry A, 116:7419-7423**.

Vöhringer-Martinez, Esteban; Duarte, Fernanda; **2012**. *How Does Pin1 Catalyze the Cis-Trans Prolyl Peptide Bond Isomerization? A QM/MM and Mean Reaction Force Study*, **Journal of Physical Chemistry B, 116:12972-12979**.

LISTADO DE PROYECTOS DE INVESTIGACIÓN EN LOS ÚLTIMOS 10 AÑOS

- ✓ 2007-2009 Beca Doctoral, Physical Chemical Graduate School Göttingen, DFG Alemania
- ✓ 2009-2011 Proyecto Postdoctoral, Alexander von Humboldt Stiftung (AvH): "Dynamics and Reactions at Interfaces", Investigador Responsable
- ✓ 2010-2012 Proyecto Postdoctoral FONDECYT 3110018: "Enzyme Catalysis of cis-trans Peptide Isomerization: A Mechanistic Study via Ab-initio Molecular Dynamics", Investigador Responsable
- ✓ 2012-2015 Proyecto Regular FONDECYT 1120093: "Mechanistic Aspects of Proton Transfer Reactions with Applications to Biomolecules and Materials Science". Coinvestigador
- ✓ 2012-2013 Proyecto CONICYT Colaboración Internacional DFG(Alemania)/Conicyt: "Estudio sobre la captura de electrones solvatados en la interfaz agua - vacío por moléculas del ámbito biológico.", Investigador Responsable
- ✓ 2012-2015 Proyecto Inicio FONDECYT 11121179: "On the Track of Enzymes' Function: New Insights from the Mean Reaction Force", Investigador Responsable.
- ✓ 2014-2017 Núcleo Milenio Procesos Químicos y Catálisis, NCI20082, Investigador Asociado.

<p>Listado de proyectos de investigación en los últimos 10 años</p>	<ul style="list-style-type: none"> • 2007-2009 Beca Doctoral, Physical Chemical Graduate School Göttingen, DFG Alemania • 2009-2011 Proyecto Postdoctoral, Alexander von Humboldt Stiftung (AvH): "Dynamics and Reactions at Interfaces", Investigador Responsable • 2010-2012 Proyecto Postdoctoral FONDECYT 3110018:"Enzyme Catalysis of cis-trans Peptide Isomerization: A Mechanistic Study via Ab-initio Molecular Dynamics", Investigador Responsable • 2012-2015 Proyecto Regular FONDECYT 1120093: "Mechanistic Aspects of Proton Transfer Reactions with Applications to Biomolecules and Materials Science". Coinvestigador • 2012-2013 Proyecto CONICYT Colaboración Internacional DFG(Alemania)/Conicyt:"Estudio sobre la captura de electrones solvatados en la interfaz agua - vacío por moléculas del ámbito biológico.", Investigador Responsable • 2012-2015 Proyecto Inicio FONDECYT 11121179: "On the Track of Enzymes' Function: New Insights from the Mean Reaction Force", Investigador Responsable. • 2014-2017 Núcleo Milenio Procesos Químicos y Catálisis, NCI20082, Investigador Asociado.
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