## André Mirtschink, PhD

**PERSONAL**


*Birth date:* 22 Nov 1985
*Birth place:* Räckelwitz, Germany
*Address:* Nano-bio Spectroscopy Group
European Theoretical Spectroscopy Facility (ETSF)
Centro Joxe Mari Korta
Avenida de Tolosa, 72
20018 Donostia-San Sebastián
Spain
*E-mail:* andre.mirtschink@gmail.com
*Web:* `http://andremirt.github.io`


**EDUCATION**

***Doctorate*** 29 Jan 2015

Department of Theoretical Chemistry,
VU University Amsterdam, The Netherlands

Supervisor: Paola Gori-Giorgi, Evert Jan Baerends
Title: Energy Density Functionals From the Strong-Interaction Limit of Density Functional Theory

***Diplom Chemiker*** 6 Jul 2009

Department of Theoretical Chemistry,
University of Technology Dresden, Germany

Supervisor: Gotthard Seifert
Topic: Reducing Empiricism in Binding Energy Calculations Within the DFTB Method

**EMPLOYMENT**

***Postdoctoral Fellow*** Sep 2015 - Mar 2015

Nano-bio Spectroscopy Group,
University of the Basque Country, Spain

***Postdoctoral Fellow*** Nov 2014 - Mar 2015

Department of Theoretical Chemistry,
VU University Amsterdam, The Netherlands

***PhD Candidate*** Nov 2010 - Oct 2014

Department of Theoretical Chemistry,
Free University Amsterdam, The Netherlands

***Leonardo Da Vinci Fellow*** Feb - Aug 2010

Quantum Chemistry and Physics Laboratory,
The National Center for Scientific Research/Paul Sabatier University, Toulouse, France

***Researcher*** Nov 2009 - Dec 2009

Department of Physics,
Federal University of Santa Catarina, Florianopolis, Brazil

***Researcher*** Sept 2009 - Oct 2009

Department of Theoretical Chemistry,
University of Technology Dresden, Germany

***Research Assistant*** Feb 2007 - Sept 2008

Department of Theoretical Chemistry,
University of Technology Dresden, Germany

***Research Assistant*** Mar 2005

Fraunhofer Institute for Electron Beam-, Plasma Technology,
Dresden, Germany

***Research Assistant*** Feb 2004

Fraunhofer Institute for Ceramic Technologies and Systems,
Dresden, Germany

**VISITING SCIENTIST**

NanoBio Spectroscopy Group, Apr 2014
The University of the Basque Country UPV/EHU, Donostia-San Sebastian, Spain

NanoBio Spectroscopy Group, Aug - Oct 2013
The University of the Basque Country UPV/EHU, Donostia-San Sebastian, Spain

Department of Theoretical Chemistry, Nov - Dec 2010
University of Science and Technology Pohang, South-Korea

**HONORS**

Leonardo Da Vinci Fellowship, European Union Feb - Aug 2010

Research fellowship, German research foundation Nov 2015 - Oct 2017

**OTHERS**

***Talks***

*"Exchange-Correlation Functionals for Strong Correlation", Department of Theoretical Chemistry, University of Technology Dresden, Germany, 19 Nov 2015, invited group seminar*

*"The Derivative Discontinuity in the Strog-Interaction Limit of Density Functional Theory", NWO-CW Study group meeting "Chemistry in Relation to Physics and Material Sciences", Veldhoven, The Netherlands, 10 Feb 2014, accepted talk*

*"Travelling the Adiabatic Connection: Towards New Exchange-Correlation Functionals", Department of Theoretical Chemistry, University of Technology Dresden, Germany, 25 May 2011, invited group seminar*

**PUBLICATIONS**

| | | | |
|---|---|---|---|
| *Number of publications:* | 10 | *Researched-ID:* | C-9355-2015 |
| *H-index:* | 5 | | |
| *Times cited:* | 57 | | |

***Top 5 publications***

1. *"The derivative discontinuity in the strong-interaction limit of density functional theory"*
   A. Mirtschink, M. Seidl and P. Gori-Giorgi
   Phys. Rev. Lett. **111**, 126402 (2013)
2. *"Density functional theory for strongly correlated dipolar ultracold gases"*
   F. Malet, A. Mirtschink, C. B. Mendl, J. Bjerlin, E. Karabulut, S. Reiman and P. Gori-Giorgi
   Phys. Rev. Lett. **115**, 033006 (2015), selected as **editor's suggestion**

3. *"Energy density functionals from the strong-coupling limit applied to the anions of the He isoelectronic series"*
   A. Mirtschink, C. J. Umrigar, J. D. Morgan III and P. Gori-Giorgi
   J. Chem. Phys. **140**, 18A532 (2014), **invited article** for special issue "Advances in Density Functional Theory"
4. *"Energy densities in the strong-interaction limit of density functional theory"*
   A. Mirtschink, M. Seidl and P. Gori-Giorgi
   J. Chem. Theory Comput. **8**, 3097 (2012)
5. *"Modeling Charge Resonance in Cationic Molecular Clusters: Combining DFT-Tight Binding with Configuration Interaction"*
   M. Rapacioli, F. Spiegelman , A. Scemama and A. Mirtschink
   J. Chem. Theory Comput. **7**, 44 (2011)

***Peer-reviewed journals***

8. *"Hydrogen molecule dissociation curve with functionals based on the strictly-correlated regime"*
   S. Vuckovic, L. O. Wagner, A. Mirtschink and P. Gori-Giorgi
   J. Chem. Theory Comput. **11**, 3153 (2015)
7. *"Density functional theory for strongly correlated dipolar ultracold gases"*
   F. Malet, A. Mirtschink, C. B. Mendl, J. Bjerlin, E. Karabulut, S. Reiman and P. Gori-Giorgi
   Phys. Rev. Lett. **115**, 033006 (2015), selected as **editor's suggestion**
6. *"Energy density functionals from the strong-coupling limit applied to the anions of the He isoelectronic series"*
   A. Mirtschink, C. J. Umrigar, J. D. Morgan III and P. Gori-Giorgi
   J. Chem. Phys. **140**, 18A532 (2014), **invited article** for special issue "Advances in Density Functional Theory"
5. *"Exchange-correlation functionals from the strongly interacting limit of DFT: Applications to model chemical systems"*
   F. Malet, A. Mirtschink, K. J. H. Giesbertz, L. O. Wagner and P. Gori-Giorgi
   Phys. Chem. Chem. Phys. **16**, 14551 (2014)
4. *"The derivative discontinuity in the strong-interaction limit of density functional theory"*
   A. Mirtschink, M. Seidl and P. Gori-Giorgi
   Phys. Rev. Lett. **111**, 126402 (2013)
3. *"Kohn-Sham density functional theory for quantum wires in arbitrary correlation regimes"*
   F. Malet, A. Mirtschink, J. C. Cremon, S. M. Reimann and P. Gori-Giorgi
   Phys. Rev. B **87**, 115146 (2013), selected as **editor's suggestion**
2. *"Energy densities in the strong-interaction limit of density functional theory"* A. Mirtschink, M. Seidl and P. Gori-Giorgi
   J. Chem. Theory Comput. **8**, 3097 (2012)
1. *"Modeling Charge Resonance in Cationic Molecular Clusters: Combining DFT-Tight Binding with Configuration Interaction"*
   M. Rapacioli, F. Spiegelman , A. Scemama and A. Mirtschink
   J. Chem. Theory Comput. **7**, 44 (2011)

***Book chapters***

1. *"Density functional theory for strongly interacting electrons"*
   F. Malet, A. Mirtschink, K. J. H. Giesbertz and P. Gori-Giorgi
   in *"Many-Electron Approaches in Physics, Chemistry and Mathematics"*, 153, Springer International Publishing, Switzerland (2014)

***Conference proceedings***

1. *"PAH-related Very Small Grains in photodissociation regions: implications from molecular simulations"*
   M. Rapacioli, F. Spiegelman, B. Joalland, A. Simon, A. Mirtschink, C. Joblin, J. Montillaud, O. Bern and D. Talbi
   EAS Publications Series, **46**, 223 (2011)