

André Mirtschink

PERSONAL

Birth date: 22 Nov 1985
Birth place: Räckelwitz, Germany
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The Netherlands
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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 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, The University of the Basque Country UPV/EHU, Donostia-San Sebastian, Spain	Apr 2014
	NanoBio Spectroscopy Group, The University of the Basque Country UPV/EHU, Donostia-San Sebastian, Spain	Aug - Oct 2013
	Department of Theoretical Chemistry, University of Science and Technology Pohang, South-Korea	Nov - Dec 2010
HONORS	Leonardo Da Vinci Fellowship, European Union, Feb - Aug 2010	
OTHERS	Talks <i>“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</i> <i>“Travelling the Adiabatic Connection: Towards New Exchange-Correlation Functionals”, Department of Theoretical Chemistry, University of Technology Dresden, Germany, 25 May 2011, invited group seminar</i>	
PUBLICATIONS	Number of publications: 10 Researched-ID: C-9355-2015 H-index: 4 Times cited: 47	
	Top publications <ol style="list-style-type: none"> 1. <i>“The derivative discontinuity in the strong-interaction limit of density functional theory”</i> A. Mirtschink, M. Seidl and P. Gori-Giorgi Phys. Rev. Lett. 111, 126402 (2013) 2. <i>“Energy density functionals from the strong-coupling limit applied to the anions of the He isoelectronic series”</i> 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” 3. <i>“Energy densities in the strong-interaction limit of density functional theory”</i> A. Mirtschink, M. Seidl and P. Gori-Giorgi J. Chem. Theory Comput. 8, 3097 (2012) 4. <i>“Modeling Charge Resonance in Cationic Molecular Clusters: Combining DFT-Tight Binding with Configuration Interaction”</i> M. Rapacioli, F. Spiegelman , A. Scemama and A. Mirtschink J. Chem. Theory Comput. 7, 44 (2011) 5. <i>“Kohn-Sham density functional theory for quantum wires in arbitrary correlation regimes”</i> F. Malet, A. Mirtschink, J. C. Cremon, S. M. Reimann and P. Gori-Giorgi Phys. Rev. B 87, 115146 (2013), highlighted as editor’s suggestion 	

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)