

C3.11 (F. Evers)

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- [C3.11:4] S. Er, M.J. van Setten, G.A. de Wijs, and G. Brocks, *First principles modeling of magnesium titanium hydrides*, [J. of Phys. Cond. Matt. **22**, 07420 \(2010\)](#)
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- [C3.11:8] F. Gebert, B. Willenberg, M.J. van Setten, E.G. Bardaji, E. Roehm, M. Fichtner, and J. Schoenes, *Polarization-dependent Raman spectroscopy of $LiBH_4$ single crystals and $Mg(BH_4)_2$ powders* [J. Raman Spec. **42**, 1796 \(2011\)](#)
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- [C3.11:10] * ‡ V. Meded, A. Bagrets, K. Fink, R. Chandrasekhar, M. Ruben, F. Evers, A. Bernard-Mantel, J.S. Seldenthuis, A. Beukman, and H.S.J. van der Zant, *Electrical control over the Fe(II) spin crossover in a single molecule: Theory and Experiment*, *Phys. Rev. B* **83**, 245415 (2011)
- [C3.11:11] A. Dasgupta, S. Bera and F. Evers, and M.J. van Setten, *Quantum Size Effects in the Atomistic Structure of Armchair-Nanoribbons*, *Phys. Rev. B* **85**, 125433 (2012)
- [C3.11:12] P. Troster, P. Schmitteckert, and F. Evers, *Transport calculations based on density functional theory: Friedel's sum rule and the Kondo effect*, *Phys. Rev. B* **85**, 115409 (2012)
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- [C3.11:14] * S. Bernadotte, F. Evers, and C. Jacob, *Plasmons in Molecules*, J. Phys. Chem. C **171**, 1863 (2013)
- [C3.11:15] M.J. van Setten, F. Weigend, and F. Evers, *The GW-Method for Quantum Chemistry Applications: Theory and Implementation*, J. Chem. Theo. Comp. **9**, 232 (2013)
- [C3.11:16] J. Wilhelm, M. Walz, M. Stendel, A. Bagrets, and F. Evers, *Ab initio simulations of scanning-tunneling-microscope images with embedding techniques and application to C58-dimers on Au(111)*, Phys. Chem. Chem. Phys. **15**, 6684 (2013)
- [C3.11:17] * N. Bajales, S. Schmaus, T. Miyamashi, W. Wulfhekel, J. Wilhelm, M. Walz, M. Stendel, A. Bagrets, F. Evers, S. Ulas, B. Kern, A. Boettcher, and M.M. Kappes, *C58 on Au(111): A scanning tunneling microscopy study*, J. Chem. Phys. **138**, 104703 (2013)
- [C3.11:18] G. Geranton, C. Seiler, A. Bagrets, L. Venkataraman, and F. Evers, *Transport properties of individual C60-molecules*, J. Chem. Phys. **139**, 23 (2013)
- [C3.11:19] T. Yelin, R. Vardamon, N. Kuritz, R. Korytar, A. Bagrets, F. Evers, L. Kronik, and O. Tal, *Atomically Wired Molecular Junctions: Connecting a Single Organic Molecule by Chains of Metal Atoms*, Nano Letters **13**, 1956 (2013)

Invited Talks at International Conferences

- F. Evers, *Transport calculations with exact exchange correlation functionals*, CECAM Workshop on Quantum transport on the molecular scale, Bremen, (13/09/2009)
- F. Evers, *Towards quantum chemistry calculations for strongly correlated systems*, Workshop on Quantum Transport in Nanoscale Molecular Systems, Telluride, (27/07/2009)
- F. Evers, *High-Spin Low-Spin transition in a single molecule and its transport signature*, Workshop on Theoretical Modeling of Transport in Nanostructures, Lausanne, (02/07/2009)
- F. Evers, *Mechanisms operating molecular switches*, Minerva International Workshop on The Science of Complexity, Eilat, Israel, (29/03/2009)
- A. Bagrets, *Fullerene-based anchoring groups for molecular electronics: insights from theory*, APS March Meeting 2010, Portland, Oregon, USA (15–19/03/2010)
- A. Bagrets, *Electron transport through van der Waals bonds and magnetoresistance at the single molecule level*, CECAM Workshop "Transport Phenomena in Molecular Nanostructures", Zurich, Switzerland, (22-25/06/2010)
- M.J. van Setten, *The GW-Method for Quantum Chemistry Applications: Theory and Implementation*, Conference on recent progress in DMFT and GW calculations (17-12/12/2012)

F. Evers, *GW-perspectives for molecular electronic-structure calculations*, International Conference Frontiers of Quantum and Mesoscopic Thermodynamics 13, Prague (29/7/2013)

F. Evers, *Ab-initio calculations of dc-current induced orbital magnetism in graphene nanoribbons*, Psi-K Workshop "Modeling Single-Molecule Junctions: Novel Spectroscopies and Control", Berlin (14/10/2013)

F. Evers, *Ab-initio transport studies: Review of fundamentals and applications to ring currents in graphene nanoribbons*, Workshop "Quantum Dynamics in Molecular and Nano-Materials: Mechanisms and Functionality", Tel Aviv (29/11/2013)