

### C3.6 (G. Schön / F. Pauly)

- [C3.6:1] ‡ H. van Zalinge, D.J. Schiffrin, A.D. Bates, E.B. Starikov, W. Wenzel, and R.J. Nichols, *Variable-temperature measurements of the single-molecule conductance of double-stranded DNA*, *Angew. Chem. Int. Ed.* **45**, 5499 (2006)
- [C3.6:2] ‡ T. Tanabe, E.B. Starikov, K. Noda, and M. Saito, *Resonant neutral-particle emission after collisions of electrons with base-stacked oligonucleotide cations in a storage ring*, *Chem. Phys. Lett.* **430**, 380 (2006)
- [C3.6:3] ‡ E.B. Starikov, T. Fujita, H. Watanabe, Y. Sengoku, S. Tanaka, and W. Wenzel, *Effects of molecular motion on charge transfer/transport through DNA duplexes with and without base pair mismatch*, *Mol. Simulat.* **32**, 759 (2006)
- [C3.6:4] ‡ E.B. Starikov, S. Tanaka, N. Kurita, Y. Sengoku, T. Natsume, A. Quintilla, and W. Wenzel, *Ballistic conductance for all-atom models of native and chemically modified DNA: a review of Kubo-formula-based approach*, In: *Modern Methods for Theoretical Physical Chemistry of Biopolymers*, Eds. E.B. Starikov, J.P. Lewis, and S. Tanaka (Elsevier, Amsterdam, 2006)
- [C3.6:5] \* ‡ C. Romeike, M. Wegewijs, W. Wenzel, M. Ruben, and H. Schoeller, *Charge-induced modulation of magnetic interactions in 2x2 metallo-organic grid-complex*, *Int. J. Quantum Chem.* **106**, 994 (2006)
- [C3.6:6] \* ‡ C. Romeike, M. Wegewijs, W. Wenzel, M. Ruben, and H. Schoeller, *Charge-switchable molecular magnet and spin-blockade of tunneling*, *Phys. Rev. B* **75**, 064404 (2007)
- [C3.6:7] B.B. Schmidt, M.H. Hettler, and G. Schön, *Influence of vibrational modes on the electronic properties of DNA*, *Phys. Rev. B* **75**, 115125 (2007)
- [C3.6:8] \* B.B. Schmidt, E.B. Starikov, M.H. Hettler, and W. Wenzel, *Vibrations in DNA: Their Influence on Transport*, in *Charge migration in DNA - Physics, Chemistry and Biology Perspectives*, Springer 2007 (ISBN 354-072-493-1), pp. 249-262
- [C3.6:9] ‡ J.K. Viljas and J.C. Cuevas, *Role of electronic structure in photo-assisted transport through atomic-sized contacts*, *Phys. Rev. B* **75**, 075406 (2007)
- [C3.6:10] ‡ J.K. Viljas, F. Pauly, and J.C. Cuevas, *Photoconductance of organic single-molecule contacts*, *Phys. Rev. B* **76**, 033403 (2007)
- [C3.6:11] ‡ S. Wohlthat, F. Pauly, J.K. Viljas, J.C. Cuevas, and G. Schön, *Ab initio study of charge transport through single oxygen molecules in atomic aluminum contacts*, *Phys. Rev. B* **76**, 075413 (2007)
- [C3.6:12] \* ‡ F. Pauly, J.K. Viljas, U. Huniar, M. Häfner, S. Wohlthat, M. Bürkle, J.C. Cuevas, and G. Schön, *Cluster-based density-functional approach to quantum transport through molecular and atomic contacts*, *New J. Phys.* **10**, 125019 (2008)
- [C3.6:13] ‡ M. Kiguchi, O. Tal, S. Wohlthat, F. Pauly, M. Krieger, D. Djukic, J.C. Cuevas, and J.M. van Ruitenbeek, *Highly conductive molecular junctions based on direct binding of benzene to platinum*, *Phys. Rev. Lett.* **101**, 046801 (2008)
- [C3.6:14] ‡ S. Wohlthat, F. Pauly, and J.R. Reimers, *The conduction properties of  $\alpha,\omega$ -diaminoalkanes and hydrazine bridging gold electrodes*, *Chem. Phys. Lett.* **454**, 284 (2008)
- [C3.6:15] ‡ F. Pauly, J.K. Viljas, J.C. Cuevas, and G. Schön, *Density-functional study of tilt-angle and temperature-dependent conductance in biphenyl-dithiol single-molecule contacts*, *Phys. Rev. B* **77**, 155312 (2008)

- [C3.6:16] ‡ F. Pauly, J.K. Viljas, and J.C. Cuevas, *Length-dependent conductance and thermopower in single-molecule junctions of dithiolated oligophenylene derivatives*, Phys. Rev. B **78**, 035315 (2008)
- [C3.6:17] ‡ S. Wohlthat, F. Pauly, and J.R. Reimers, *Two-dimensional, phenanthroline-based, extended  $\pi$ -conjugated molecules for single-molecule conduction*, J. Phys-Condens. Mat. **20**, 295208 (2008)
- [C3.6:18] ‡ J.K. Viljas, F. Pauly, and J.C. Cuevas, *Modeling elastic and photoassisted transport in organic molecular wires: Length dependence and current-voltage characteristics*, Phys. Rev. B **77**, 155119 (2008)
- [C3.6:19] ‡ A.V. Danilov, P. Hedegard, D.S. Golubev, T. Bjornholm, and S.E. Kubatkin, *Nanoelectromechanical switch operating by tunneling of an entire C60 molecule*, Nano Lett. **8**, 2393 (2008)
- [C3.6:20] ‡ J.J. Kwiatkowski, J. Nelson, H. Li, J.L. Bredas, W. Wenzel, and C. Lennartz, *Simulating charge transport in tris(8-hydroxyquinoline) aluminium (Alq3)*, Phys. Chem. Chem. Phys. **10**, 1852 (2008)
- [C3.6:21] B.B. Schmidt, M.H. Hettler, and G. Schön, *Non-equilibrium polaron hopping transport through DNA*, Phys. Rev. B **77**, 165337 (2008)
- [C3.6:22] E.B. Starikov, A. Quintilla, K.H. Lee, and W. Wenzel, *Conformational dependence of DNA ballistic conductivity*, J. Chem. Phys. **129**, 131101 (2008)
- [C3.6:23] ‡ E.B. Starikov, A. Quintilla, C. Nganou, K.H. Lee, G. Cuniberti, and W. Wenzel, *Single-molecule DNA conductance in water solutions: Role of DNA low-frequency dynamics*, Chem. Phys. Lett. **467**, 369 (2009)
- [C3.6:24] B.B. Schmidt, M.H. Hettler, and G. Schön, *Charge correlations in polaron hopping through molecules*, Phys. Rev. B **82**, 155113 (2010)
- [C3.6:25] ‡ L.A. Zotti, T. Kirchner, J.C. Cuevas, F. Pauly, T. Huhn, E. Scheer, and A. Erbe, *Revealing the role of anchoring groups in the electrical conduction through single-molecule junctions*, Small **6**, 1529 (2010)
- [C3.6:26] \* ‡ A. Mishchenko, D. Vonlanthen, V. Meded, M. Bürkle, C. Li, I.V. Pobelov, A. Bagrets, J.K. Viljas, F. Pauly, F. Evers, M. Mayor, and T. Wandlowski, *Influence of conformation on conductance of biphenyl-dithiol single-molecule contacts*, Nano Lett. **10**, 156 (2010)
- [C3.6:27] \* ‡ A. Mishchenko, L.A. Zotti, D. Vonlanthen, M. Bürkle, F. Pauly, J.C. Cuevas, M. Mayor, and T. Wandlowski, *Single-Molecule Junctions Based on Nitrile-Terminated Biphenyls: A Promising New Anchoring Group*, J. Am. Chem. Soc. **133**, 184 (2011)
- [C3.6:28] Y. Kim, T.J. Hellmuth, M. Bürkle, F. Pauly, and E. Scheer, *Characteristics of amine-ended and thiol-ended alkane single-molecule junctions revealed by inelastic electron tunneling spectroscopy*, ACS Nano **5**, 4104 (2011)
- [C3.6:29] ‡ L.A. Zotti, M. Bürkle, Y.J. Dappe, F. Pauly, and J.C. Cuevas, *Electronic transport through single noble gas atoms*, Phys. Rev. B **84**, 193404 (2011)
- [C3.6:30] \* ‡ M. Bürkle, J. K. Viljas, A. Mishchenko, D. Vonlanthen, G. Schön, M. Mayor, T. Wandlowski, and F. Pauly, *Conduction mechanisms in biphenyl-dithiol single-molecule junctions*, arXiv:1109.0273 [cond-mat.mes-hall]