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Tuned Range-Separated Density Functional Theory and Dyson Orbital Formalism for Photoelectron Spectra

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Abstract

© 2018 American Chemical Society. Photoelectron spectroscopy represents a valuable tool to analyze structural and dynamical changes in molecular systems. Comprehensive interpretation of experimental data requires, however, involvement of reliable theoretical modeling. In this work, we present a protocol based on the combination of well-established linear-response time-dependent density functional theory and Dyson orbital formalism for the accurate prediction of both ionization energies and intensities. Essential here is the utilization of the optimally tuned range-separated hybrid density functionals, improving the ionization potentials not only of frontier but also of the deeper lying orbitals. In general, the protocol provides accurate results as illustrated by comparison to experiments for several gas-phase molecules, belonging to different classes. Further, we analyze possible pitfalls of this approach and, namely, discuss the ambiguities in the choice of optimal range-separation parameters, the influence of the stability of the ground state, and the spin contamination issues as possible sources of inaccuracies.

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References

[1] Hüfner, Stefan. Photoelectron Spectroscopy; Springer: Berlin, 1996.

[2] Winter, B.; Faubel, M. Photoemission from Liquid Aqueous Solutions. Chem. Rev. 2006, 106, 1176-1211, 10.1021/cr040381p

[3] Koopmans, T. Über die Zuordnung von Wellenfunktionen und Eigenwerten zu den einzelnen Elektronen eines Atoms. Physica 1934, 1, 104-113, 10.1016/S0031-8914(34)90011-2

[4] Almbladh, C.-O.; von Barth, U. Exact Results for the Charge and Spin Densities, Exchange-Correlation Potentials, and Density-Functional Eigenvalues. Phys. Rev. B: Condens. Matter Mater. Phys. 1985, 31, 3231-3244, 10.1103/PhysRevB.31.3231

[5] Perdew, J. P.; Parr, R. G.; Levy, M.; Balduz, J. L. Density-Functional Theory for Fractional Particle Number: Derivative Discontinuities of the Energy. Phys. Rev. Lett. 1982, 49, 1691-1694, 10.1103/PhysRevLett.49.1691

[6] Chong, D. P.; Gritsenko, O. V.; Baerends, E. J. Interpretation of the Kohn-Sham Orbital Energies as Approximate Vertical Ionization Potentials. J. Chem. Phys. 2002, 116, 1760-1772, 10.1063/1.1430255

[7] Egger, D. A.; Weissman, S.; Refaely-Abramson, S.; Sharifzadeh, S.; Dauth, M.; Baer, R.; Kümmel, S.; Neaton, J. B.; Zojer, E.; Kronik, L. Outer-Valence Electron Spectra of Prototypical Aromatic Heterocycles from an Optimally Tuned Range-Separated Hybrid Functional. J. Chem. Theory Comput. 2014, 10, 1934-1952, 10.1021/ct400956h

[8] Yepes, D.; Seidel, R.; Winter, B.; Blumberger, J.; Jaque, P. Photoemission Spectra and Density Functional Theory Calculations of 3d Transition Metal-Aqua Complexes (Ti-Cu) in Aqueous Solution. J. Phys. Chem. B 2014, 118, 6850-6863, 10.1021/jp5012389

[9] Brumboiu, I. E.; Prokopiou, G.; Kronik, L.; Brena, B. Valence Electronic Structure of Cobalt Phthalocyanine from an Optimally Tuned Range-Separated Hybrid Functional. J. Chem. Phys. 2017, 147, 044301, 10.1063/1.4993623

[10] Gao, C.-Z.; Wopperer, P.; Dinh, P. M.; Suraud, E.; Reinhard, P.-G. On the Dynamics of Photo-Electrons in C. J. Phys. B: At., Mol. Opt. Phys. 2015, 48, 105102, 10.1088/0953-4075/48/10/105102

[11] Von Niessen, W.; Schirmer, J.; Cederbaum, L. S. Computational Methods for the One-Particle Green's Function. Comput. Phys. Rep. 1984, 1, 57-125, 10.1016/0167-7977(84)90002-9

[12] Schirmer, J.; Cederbaum, L. S.; Walter, O. New Approach to the One-Particle Green's Function for Finite Fermi Systems. Phys. Rev. A: At., Mol., Opt. Phys. 1983, 28, 1237-1259, 10.1103/PhysRevA.28.1237

[13] Kadanoff, L. P.; Baym, G. Quantum Statistical Mechanics: Green's Function Method in Equilibrium and Nonequilibrium Problems; Addison-Wesley: Redwood City, CA, USA, 1989.

[14] Pohl, A.; Reinhard, P.-G.; Suraud, E. Towards Single-Particle Spectroscopy of Small Metal Clusters. Phys. Rev. Lett. 2000, 84, 5090-5093, 10.1103/PhysRevLett.84.5090

[15] Bachau, H.; Cormier, E.; Decleva, P.; Hansen, J. E.; Martín, F. Applications of B-Splines in Atomic and Molecular Physics. Rep. Prog. Phys. 2001, 64, 1815-1943, 10.1088/0034-4885/64/12/205

[16] Colle, R.; Embriaco, D.; Massini, M.; Simonucci, S.; Taioli, S. Ab Initio Calculation of the C1s Photoelectron Spectrum of CH. Nucl. Instrum. Methods Phys. Res., Sect. B 2004, 213, 65-70, 10.1016/S0168-583X(03)0153--0

[17] Ponzi, A.; Sapunar, M.; Angeli, C.; Cimiraglia, R.; Došlić, N.; Decleva, P. Photoionization of Furan from the Ground and Excited Electronic States. J. Chem. Phys. 2016, 144, 084307, 10.1063/1.4941608

[18] Tao, L.; McCurdy, C. W.; Rescigno, T. N. Grid-Based Methods for Diatomic Quantum Scattering Problems: A Finite-Element Discrete-Variable Representation in Prolate Spheroidal Coordinates. Phys. Rev. A: At., Mol., Opt. Phys. 2009, 79, 012719, 10.1103/PhysRevA.79.012719

[19] Larsson, H. R.; Bauch, S.; Sørensen, S.; Bonitz, M. Correlation Effects in Strong-Field Ionization of Heteronuclear Diatomic Molecules. Phys. Rev. A: At., Mol., Opt. Phys. 2016, 93, 013426, 10.1103/PhysRevA.93.013426

[20] Dauth, M.; Graus, M.; Schelter, I.; Wießner, M.; Schöll, A.; Reinert, F.; Kümmel, S. Perpendicular Emission, Dichroism, and Energy Dependence in Angle-Resolved Photoemission: The Importance of The Final State. Phys. Rev. Lett. 2016, 117, 183001, 10.1103/PhysRevLett.117.183001

[21] Marante, C.; Klinker, M.; Corral, I.; González-Vázquez, J.; Argenti, L.; Martín, F. Hybrid-Basis Close-Coupling Interface to Quantum Chemistry Packages for the Treatment of Ionization Problems. J. Chem. Theory Comput. 2017, 13, 499-514, 10.1021/acs.jctc.6b00907

[22] De Giovannini, U.; Hübener, H.; Rubio, A. A First-Principles Time-Dependent Density Functional Theory Framework for Spin and Time-Resolved Angular-Resolved Photoelectron Spectroscopy in Periodic Systems. J. Chem. Theory Comput. 2017, 13, 265-273, 10.1021/acs.jctc.6b00897

[23] Pickup, B. T. On the Theory of Fast Photoionization Processes. Chem. Phys. 1977, 19, 193-208, 10.1016/0301-0104(77)85131-8

[24] Oana, C. M.; Krylov, A. I. Cross Sections and Photoelectron Angular Distributions in Photodetachment from Negative Ions Using Equation-of-Motion Coupled-Cluster Dyson Orbitals. J. Chem. Phys. 2009, 131, 124114, 10.1063/1.3231143

[25] Decleva, P.; Fronzoni, G.; Kivimäki, A.; álvarez Ruiz, J.; Svensson, S. Shake-up Transitions in S 2p, S 2s and F 1s Photoionization of the SF Molecule. J. Phys. B: At., Mol. Opt. Phys. 2009, 42, 055102, 10.1088/0953-4075/42/5/055102

[26] Grell, G.; Bokarev, S. I.; Winter, B.; Seidel, R.; Aziz, E. F.; Aziz, S. G.; Kühn, O. Multi-Reference Approach to the Calculation of Photoelectron Spectra Including Spin-Orbit Coupling. J. Chem. Phys. 2015, 143, 074104, 10.1063/1.4928511

[27] Kronik, L.; Kümmel, S. In First Principles Approaches to Spectroscopic Properties of Complex Materials; Di Valentin, C., Botti, S., Cococcioni, M., Eds.; Springer: Berlin, Heidelberg, 2014; Vol. 347, pp 137-191.

[28] Jones, R. O. Density Functional Theory: Its Origins, Rise to Prominence, and Future. Rev. Mod. Phys. 2015, 87, 897-923, 10.1103/RevModPhys.87.897

[29] Leang, S. S.; Zahariev, F.; Gordon, M. S. Benchmarking the Performance of Time-Dependent Density Functional Methods. J. Chem. Phys. 2012, 136, 104101, 10.1063/1.3689445

[30] Baer, R.; Livshits, E.; Salzner, U. Tuned Range-Separated Hybrids in Density Functional Theory. Annu. Rev. Phys. Chem. 2010, 61, 85-109, 10.1146/annurev.physchem.012809.103321

[31] Kümmel, S.; Kronik, L. Orbital-Dependent Density Functionals: Theory and Applications. Rev. Mod. Phys. 2008, 80, 3-60, 10.1103/RevModPhys.80.3

[32] Savin, A. Recent Advances in Computational Chemistry; World Scientific: Singapore, 1995; Vol. 1, pp 129-153.

[33] Refaely-Abramson, S.; Sharifzadeh, S.; Govind, N.; Autschbach, J.; Neaton, J. B.; Baer, R.; Kronik, L. Quasiparticle Spectra from a Nonempirical Optimally Tuned Range-Separated Hybrid Density Functional. Phys. Rev. Lett. 2012, 109, 226405, 10.1103/PhysRevLett.109.226405

[34] Gozem, S.; Gunina, A. O.; Ichino, T.; Osborn, D. L.; Stanton, J. F.; Krylov, A. I. Photoelectron Wave Function in Photoionization: Plane Wave or Coulomb Wave?. J. Phys. Chem. Lett. 2015, 6, 4532-4540, 10.1021/acs.jpclett.5b01891

[35] Walter, M.; Häkkinen, H. Photoelectron Spectra from First Principles: From the Many-Body to the Single-Particle Picture. New J. Phys. 2008, 10, 043018, 10.1088/1367-2630/10/4/043018

[36] Humeniuk, A.; Wohlgemuth, M.; Suzuki, T.; Mitrić, R. Time-Resolved Photoelectron Imaging Spectra from Non-Adiabatic Molecular Dynamics Simulations. J. Chem. Phys. 2013, 139, 134104, 10.1063/1.4820238

[37] Onida, G.; Reining, L.; Rubio, A. Electronic Excitations: Density-Functional versus Many-Body Green's-Function Approaches. Rev. Mod. Phys. 2002, 74, 601-659, 10.1103/RevModPhys.74.601

[38] Hirata, S.; Head-Gordon, M. Time-Dependent Density Functional Theory within the Tamm-Dancoff Approximation. Chem. Phys. Lett. 1999, 314, 291-299, 10.1016/S0009-2614(99)01149-5

[39] Åberg, T. Theory of X-Ray Satellites. Phys. Rev. 1967, 156, 35-41, 10.1103/PhysRev.156.35

[40] Ipatov, A.; Cordova, F.; Doriol, L. J.; Casida, M. E. Excited-State Spin-Contamination in Time-Dependent Density-Functional Theory for Molecules with Open-Shell Ground States. J. Mol. Struct.: THEOCHEM 2009, 914, 60-73, 10.1016/j.theochem.2009.07.036

[41] Wittbrodt, J. M.; Schlegel, H. B. Some Reasons Not to Use Spin Projected Density Functional Theory. J. Chem. Phys. 1996, 105, 6574-6577, 10.1063/1.472497

[42] Peach, M. J. G.; Tozer, D. J. Overcoming Low Orbital Overlap and Triplet Instability Problems in TDDFT. J. Phys. Chem. A 2012, 116, 9783-9789, 10.1021/jp308662x

[43] Casida, M.; Huix-Rotllant, M. Progress in Time-Dependent Density-Functional Theory. Annu. Rev. Phys. Chem. 2012, 63, 287-323, 10.1146/annurev-physchem-032511-143803

[44] Peach, M. J. G.; Williamson, M. J.; Tozer, D. J. Influence of Triplet Instabilities in TDDFT. J. Chem. Theory Comput. 2011, 7, 3578-3585, 10.1021/ct200651r

[45] Leininger, T.; Stoll, H.; Werner, H.-J.; Savin, A. Combining Long-Range Configuration Interaction with Short-Range Density Functionals. Chem. Phys. Lett. 1997, 275, 151-160, 10.1016/S0009-2614(97)00758-6

[46] Yanai, T.; Tew, D. P.; Handy, N. C. A New Hybrid Exchange-Correlation Functional Using the Coulomb-Attenuating Method (CAM-B3LYP). Chem. Phys. Lett. 2004, 393, 51-57, 10.1016/j.cplett.2004.06.011

[47] Tawada, Y.; Tsuneda, T.; Yanagisawa, S.; Yanai, T.; Hirao, K. A Long-Range-Corrected Time-Dependent Density Functional Theory. J. Chem. Phys. 2004, 120, 8425-8433, 10.1063/1.1688752

[48] Song, J.-W.; Hirosawa, T.; Tsuneda, T.; Hirao, K. Long-Range Corrected Density Functional Calculations of Chemical Reactions: Redetermination of Parameter. J. Chem. Phys. 2007, 126, 154105, 10.1063/1.2721532

[49] Refaely-Abramson, S.; Baer, R.; Kronik, L. Fundamental and Excitation Gaps in Molecules of Relevance for Organic Photovoltaics from an Optimally Tuned Range-Separated Hybrid Functional. Phys. Rev. B: Condens. Matter Mater. Phys. 2011, 84, 075144, 10.1103/PhysRevB.84.075144

[50] Borpuzari, M. P.; Kar, R. A New Nonempirical Tuning Scheme with Single Self-Consistent Field Calculation: Comparison with Global and IP-Tuned Range-Separated Functional. J. Comput. Chem. 2017, 38, 2258-2267, 10.1002/jcc.24876

[51] Stein, T.; Kronik, L.; Baer, R. Reliable Prediction of Charge Transfer Excitations in Molecular Complexes Using Time-Dependent Density Functional Theory. J. Am. Chem. Soc. 2009, 131, 2818-2820, 10.1021/ja8087482

[52] Bokareva, O. S.; Grell, G.; Bokarev, S. I.; Kühn, O. Tuning Range-Separated Density Functional Theory for Photocatalytic Water Splitting Systems. J. Chem. Theory Comput. 2015, 11, 1700-1709, 10.1021/acs.jctc.5b00068

[53] Bokarev, S. I.; Bokareva, O. S.; Kühn, O. A Theoretical Perspective on Charge Transfer in Photocatalysis. The Example of Ir-Based Systems. Coord. Chem. Rev. 2015, 304-305, 133-145, 10.1016/j.ccr.2014.12.016

[54] Körzdörfer, T.; Sears, J. S.; Sutton, C.; Brédas, J.-L. Long-Range Corrected Hybrid Functionals for π-Conjugated Systems: Dependence of the Range-Separation Parameter on Conjugation Length. J. Chem. Phys. 2011, 135, 204107, 10.1063/1.3663856

[55] Karolewski, A.; Kronik, L.; Kümmel, S. Using Optimally Tuned Range Separated Hybrid Functionals in Ground-State Calculations: Consequences and Caveats. J. Chem. Phys. 2013, 138, 204115, 10.1063/1.4807325

[56] Srebro, M.; Autschbach, J. Tuned Range-Separated Time-Dependent Density Functional Theory Applied to Optical Rotation. J. Chem. Theory Comput. 2012, 8, 245-256, 10.1021/ct200764g

[57] Srebro, M.; Autschbach, J. Does a Molecule-Specific Density Functional Give an Accurate Electron Density? The Challenging Case of the CuCl Electric Field Gradient. J. Phys. Chem. Lett. 2012, 3, 576-581, 10.1021/jz201685r

[58] Autschbach, J.; Srebro, M. Delocalization Error and ''Functional Tuning'' in Kohn-Sham Calculations of Molecular Properties. Acc. Chem. Res. 2014, 47, 2592-602, 10.1021/ar500171t

[59] Livshits, E.; Baer, R. A Density Functional Theory for Symmetric Radical Cations from Bonding to Dissociation. Phys. Chem. Chem. Phys. 2007, 9, 2932-41, 10.1039/b617919c

[60] Stein, T.; Kronik, L.; Baer, R. Prediction of Charge-Transfer Excitations in Coumarin-Based Dyes Using a Range-Separated Functional Tuned from First Principles. J. Chem. Phys. 2009, 131, 244119, 10.1063/1.3269029

[61] Mori-Sánchez, P.; Cohen, A. J.; Yang, W. Localization and Delocalization Errors in Density Functional Theory and Implications for Band-Gap Prediction. Phys. Rev. Lett. 2008, 100, 146401, 10.1103/PhysRevLett.100.146401

[62] Iikura, H.; Tsuneda, T.; Yanai, T.; Hirao, K. A Long-Range Correction Scheme for Generalized-Gradien--Approximation Exchange Functionals. J. Chem. Phys. 2001, 115, 3540-3544, 10.1063/1.1383587

[63] Bauernschmitt, R.; Ahlrichs, R. Stability Analysis for Solutions of the Closed Shell Kohn-Sham Equation. J. Chem. Phys. 1996, 104, 9047-9052, 10.1063/1.471637

[64] Weigend, F.; Ahlrichs, R. Balanced Basis Sets of Split Valence, Triple Zeta Valence and Quadruple Zeta Valence Quality for H to Rn: Design and Assessment of Accuracy. Phys. Chem. Chem. Phys. 2005, 7, 3297-3305, 10.1039/b508541a

[65] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision D.01; Gaussian: Wallingford, CT, USA, 2009.

[66] Valiev, M.; Bylaska, E. J.; Govind, N.; Kowalski, K.; Straatsma, T. P.; Van Dam, H. J. J.; Wang, D.; Nieplocha, J.; Apra, E.; Windus, T. L.; de Jong, W. A. NWChem: A Comprehensive and Scalable Open-Source Solution for Large Scale Molecular Simulations. Comput. Phys. Commun. 2010, 181, 1477-1489, 10.1016/j.cpc.2010.04.018

[67] Landau, L. D.; Lifshitz, E. M. Quantum Mechanics: Non-Relativistic Theory; Pergamon: Oxford, U.K., 1977.

[68] Gozem, S.; Krylov, A. I. ezDyson; iOpenShell, University of Southern California: Los Angeles, http://iopenshell.usc.edu/downloads/ezdyson, 2017.

[69] Dauth, M.; Caruso, F.; Kümmel, S.; Rinke, P. Piecewise Linearity in the GW Approximation for Accurate Quasiparticle Energy Predictions. Phys. Rev. B: Condens. Matter Mater. Phys. 2016, 93, 121115, 10.1103/PhysRevB.93.121115

[70] Vetter, K.; Proch, S.; Ganteför, G. F.; Behera, S.; Jena, P. Hydrogen Mimicking the Properties of Coinage Metal Atoms in Cu and Ag Monohydride Clusters. Phys. Chem. Chem. Phys. 2013, 15, 21007, 10.1039/c3cp53561d

[71] Ho, J.; Ervin, K. M.; Lineberger, W. C. Photoelectron Spectroscopy of Metal Cluster Anions: Cu, Ag, and Au. J. Chem. Phys. 1990, 93, 6987-7002, 10.1063/1.459475

[72] Taylor, K. J.; Pettiette-Hall, C. L.; Cheshnovsky, O.; Smalley, R. E. Ultraviolet Photoelectron Spectra of Coinage Metal Clusters. J. Chem. Phys. 1992, 96, 3319-3329, 10.1063/1.461927

[73] Leopold, D. G.; Ho, J.; Lineberger, W. C. Photoelectron Spectroscopy of Mass-selected Metal Cluster Anions. I. Cu, n = 1-10. J. Chem. Phys. 1987, 86, 1715-1726, 10.1063/1.452170

[74] Winter, B.; Weber, R.; Widdra, W.; Dittmar, M.; Faubel, M.; Hertel, I. V. Full Valence Band Photoemission from Liquid Water Using EUV Synchrotron Radiation. J. Phys. Chem. A 2004, 108, 2625-2632, 10.1021/jp030263q

[75] Liu, S.-Y.; Alnama, K.; Matsumoto, J.; Nishizawa, K.; Kohguchi, H.; Lee, Y.-P.; Suzuki, T. He I Ultraviolet Photoelectron Spectroscopy of Benzene and Pyridine in Supersonic Molecular Beams Using Photoelectron Imaging. J. Phys. Chem. A 2011, 115, 2953-2965, 10.1021/jp1098574

[76] Richardson, N. V.; Weinberger, P. The Electronic Structure of the S Molecule. J. Electron Spectrosc. Relat. Phenom. 1975, 6, 109-116, 10.1016/0368-2048(75)80003-X

[77] Boschi, R.; Schmidt, W. The Photoelectron Spectrum and Structure of Sulfur in the Gas Phase at 140 °C. Inorg. Nucl. Chem. Lett. 1973, 9, 643-648, 10.1016/0020-1650(73)80172-2

[78] Berkowitz, J.; Lifshitz, C. Photoionization of High-Temperature Vapors. II. Sulfur Molecular Species. J. Chem. Phys. 1968, 48, 4346-4350, 10.1063/1.1667997

[79] Rosinger, W.; Grade, M.; Hirschwald, W. Electron Impact Induced Excitation Processes Involving the Sulfur Clusters S to S. Ber. Bunsenges. Phys. Chem. 1983, 87, 536-542, 10.1002/bbpc.19830870616

[80] Berkowitz, J.; Chupka, W. A. Vaporization Processes Involving Sulfur. J. Chem. Phys. 1964, 40, 287-295, 10.1063/1.1725111

[81] Hagemann, R. Determination de La Chaleur de Formation de SO Par Spectrometrie de Masse. C. R. Chim. 1962, 255, 1102

[82] Rau, H.; Kutty, T.; Guedes De Carvalho, J. Thermodynamics of Sulphur Vapour. J. Chem. Thermodyn. 1973, 5, 833-844, 10.1016/S0021-9614(73)80045-X

[83] Engel, N.; Bokarev, S. I.; Moguilevski, A.; Raheem, A. A.; Al-Obaidi, R.; Möhle, T.; Grell, G.; Siefermann, K. R.; Abel, B.; Aziz, S. G.; Kühn, O.; Borgwardt, M.; Kiyan, I. Y.; Aziz, E. F. Light-Induced Relaxation Dynamics of the Ferricyanide Ion Revisited by Ultrafast XUV Photoelectron Spectroscopy. Phys. Chem. Chem. Phys. 2017, 19, 14248-14255, 10.1039/C7CP01288H

[84] Raheem, A. A.; Wilke, M.; Borgwardt, M.; Engel, N.; Bokarev, S. I.; Grell, G.; Aziz, S. G.; Kühn, O.; Kiyan, I. Y.; Merschjann, C.; Aziz, E. F. Ultrafast Kinetics of Linkage Isomerism in Na [Fe(CN)NO] Aqueous Solution Revealed by Time-Resolved Photoelectron Spectroscopy. Struct. Dyn. 2017, 4, 044031, 10.1063/1.4990567

[85] Moguilevski, A.; Wilke, M.; Grell, G.; Bokarev, S. I.; Aziz, S. G.; Engel, N.; Raheem, A. A.; Kühn, O.; Kiyan, I. Y.; Aziz, E. F. Ultrafast Spin Crossover in [Fe(bpy)]: Revealing Two Competing Mechanisms by Extreme Ultraviolet Photoemission Spectroscopy. ChemPhysChem 2017, 18, 465-469, 10.1002/cphc.201601396

[86] Myneni, H.; Casida, M. E. On the Calculation of S for Electronic Excitations in Time-Dependent Density-Functional Theory. Comput. Phys. Commun. 2017, 213, 72-91, 10.1016/j.cpc.2016.12.011

[87] Yamaguchi, K.; Jensen, F.; Dorigo, A.; Houk, K. A Spin Correction Procedure for Unrestricted Hartree-Fock and Møller-Plesset Wavefunctions for Singlet Diradicals and Polyradicals. Chem. Phys. Lett. 1988, 149, 537-542, 10.1016/0009-2614(88)80378-6

[88] Hratchian, H. P. Communication: An Efficient Analytic Gradient Theory for Approximate Spin Projection Methods. J. Chem. Phys. 2013, 138, 101101, 10.1063/1.4795429