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Education

Ph.D. in Chemistry, **Massachusetts Institute of Technology**, Cambridge, MA, 2006.

M.S. in Chemistry, **National Taiwan University**, Taipei, Taiwan, 1997.

B.S. in Chemistry, **National Taiwan University**, Taipei, Taiwan, 1995.

Professional Experience

NTU Department of Chemistry, Taipei, Taiwan. (July 2015 - present)
Associate Professor

NTU Department of Chemistry, Taipei, Taiwan. (July 2009 - July 2015)
Assistant Professor

U.C. Berkeley Department of Chemistry, Berkeley, CA. (March 2006 - June 2009)
Postdoctoral Fellow with Professor Graham R. Fleming.

MIT Department of Chemistry, Cambridge, MA. (September 2000 - February 2006)
Graduate Research Associate with Professor Robert J. Silbey.

Research Interests

Non-equilibrium statistical mechanics and quantum dynamics of condensed-phase molecular systems. Dynamics of photosynthetic light harvesting. Photon-induced chemical dynamics. Theories for ultrafast nonlinear spectroscopy. Theoretical multi-scale modeling of organic optoelectronic nano-materials.

Awards

Outstanding Teaching Award, National Taiwan University (2015); FAOS Outstanding Young Scholar Scholarship (2010-2014); 2013 Promising Scientist Award of CMOA (Prix d'Incitation Scientifique du CMOA, 2013); Excellence in Teaching Award, National Taiwan University (2011, 2012, 2013, and 2014); The Distinguished Lectureship Award of the CSJ Asian International Symposium (2011).

List of Publications

- H.-H. Teh, B.-Y. Jin, and Y.-C. Cheng, "Frozen-mode small polaron quantum master equation with variational bound for excitation energy transfer in molecular aggregates" *J. Chem. Phys.*, **150**, 224110 (2019).
- Y.-C. Huang and Y.-C. Cheng, "C-N Bond Rotation Controls Photoinduced Electron Transfer in an Aminostyrene-Stilbene Donor-Acceptor System" *J. Phys. Chem. A*, **123**, 4333 (2019).
- W.-C. Chen, P.-T. Chou, and Y.-C. Cheng, "Low Internal Reorganization Energy of the Metal-Metal-to-Ligand Charge Transfer Emission in Dimeric Pt(II) Complexes" *J. Phys. Chem. C*, **123**, 10225 (2019).
- S.-T. Hsieh, L. Zhang, D.-W. Ye, X. Huang, and Y.-C. Cheng, "A theoretical study on the dynamics of light harvesting in the dimeric photosystem II core complex: regulation and robustness of energy transfer pathways" *Faraday Discuss.* **216**, 94 (2019).
- B.-X. Wang, M.-J. Tao, Q. Ai, T. Xin, N. Lambert, D. Ruan, Y.-C. Cheng, F. Nori, F.-G. Deng, and G.-L. Long, "Efficient quantum simulation of photosynthetic light harvesting" *Npj Quantum Information* **4**, 52 (2018).
- P.-J. Wu, Y.-F. Wang, W.-C. Chen, C.-W. Wang, Joy Cheng, Vencent Chang, C.-Y. Chang, John Lin, Y.-C. Cheng, "Nanoscale inhomogeneity and photoacid generation dynamics in extreme ultraviolet resist materials.", Proc. SPIE 10586, Advances in Patterning Materials and Processes XXXV, 105861O (March 2018); doi: 10.1117/12.2316308. (SPIE Advanced Lithography 2018 Jeffrey Byers Memorial Award)
- Y.-F. Wang, Cheng and Y.-C. Cheng, "Molecular electrostatic potential on the proton-donating atom as a theoretical descriptor of excited state acidity" *Phys. Chem. Chem. Phys.*, **20**, 4351 (2018).
- J. Feng, C.-W. Tseng, T.W. Chen, X. Leng, H.B. Yin, Y.-C. Cheng, M. Rohlfing and Y.-C. Ma, "A new energy transfer channel from carotenoids to chlorophylls in purple bacteria" *Nat. Comm.*, **8**, 1 (2017).
- K.-H. Yu, S.-L. Huang, Y.-H. Liu, Y. Wang, S.-T. Liu, Y.-C. Cheng, Y.-F. Lin, and J.-T. Chen, "Kinetics, Mechanism and Theoretical Studies of Norbornene-Ethylene Alternating Copolymerization Catalyzed by Organopalladium(II) Complexes Bearing Hemilabile α -Amino-pyridine" *Molecules* **22**, 1095 (2017).
- H.-H. Teh and Y.-C. Cheng, "On the accuracy of the LSC-IVR approach for excitation energy transfer in molecular aggregates" *J. Chem. Phys.*, **146**, 144105 (2017).

- M.-J. Tao, Q. Ai, F.-G. Deng and Y.-C. Cheng, "Proposal for probing energy transfer pathway by single-molecule pump-dump experiment" *Sci. Rep.*, **6**, 27535 (2016).
- H.-B. Chen, N. Lambert, Y.-C. Cheng, Y.-N. Chen, F. Nori, "Using non-Markovian measures to evaluate quantum master equations for photosynthesis" *Sci. Rep.*, **5**, 12753 (2015).
- C.-W. Tung, Y.-Y. Hsu, Y.-P. Shen, Y. Zheng, T.-S. Chan, H.-S. Sheu, Y.-C. Cheng, H.-M. Chen, "Reversible adapting layer produces robust single-crystal electrocatalyst for oxygen evolution" *Nat. Comm.*, **6**, 8106 (2015).
- Y. Chang and Y.-C. Cheng, "On the Accuracy of Coherent Modified Redfield Theory in Simulating Excitation Energy Transfer Dynamics" *J. Chem. Phys.*, **142**, 034109 (2015).
- Y.-H. Hwang-Fu, W. Chen, Y.-C. Cheng, "A Coherent Modified Redfield Theory for Excitation Energy Transfer in Molecular Aggregates" *Chem. Phys.*, **447**, 46 (2015).
- S.-C. Luo, Y. Khin, S.-J. Huang, Y. Yang, T.-Y. Hou, Y.-C. Cheng, H. M. Chen, Y.-Y. Chin, C.-T. Chen, H.-J. Lin, J. K.-H. Tang, J. C. C. Chan, "Probing the spatial organization of Bacteriochlorophyll c by solid-state nuclear magnetic resonance" *Biochemistry*, **53**, 5515 (2014).
- Y.-H. Ho, M.-C. Chang, K.-H. Yu, Y.-H. Liu, Y. Wang, Y.-C. Cheng, J.-T. Chen, "CO₂ fixation by dicopper(II) complexes in hypodentate framework of N₈O₂", *Dalton Trans.*, **43**, 6287 (2014).
- Q. Ai, Y.-J. Fan, B.-Y. Jin, Y.-C. Cheng, "An efficient quantum jump method for coherent energy transfer dynamics in photosynthetic systems under the influence of laser fields", *New J. Phys.*, **16**, 053033 (2014).
- H.-T. Chang, P.-P. Zhang, Y.-C. Cheng, "Criteria for the accuracy of small polaron quantum master equation in simulating excitation energy transfer dynamics", *J. Chem. Phys.*, **139**, 224112 (2013).
- Q. Ai, T.-C. Yen, B.-Y. Jin, Y.-C. Cheng, "Clustered geometries exploiting quantum coherence effects for efficient energy transfer in light harvesting", *J. Phys. Chem. Lett.*, **4**, 2577 (2013).
- C.-K. Lin, Y.-F. Wang, Y.-C. Cheng, J.-S. Yang, "Multisite constrained model of trans-4-(N,N-Dimethylamino)-4'-nitrostilbene for structural elucidation of radiative and nonradiative excited states", *J. Phys. Chem. A*, **117**, 3158 (2013).
- S.J. Jang, Y.-C. Cheng, "Resonance energy flow dynamics of coherently delocalized excitons in biological and macromolecular systems: Recent theoretical advances and open issues", *WIREs Computat. Mol. Sci.*, **3**, 84 (2013).
- N. Lambert, Y.-N. Chen, Y.-C. Cheng, C.-M. Li, G.-Y. Chen, F. Nori, "Quantum biology", *Nat. Phys.*, **9**, 10 (2013).
- H.-T. Chang, Y.-C. Cheng, "Coherent versus incoherent excitation energy transfer in molecular systems", *J. Chem. Phys.*, **137**, 165103 (2012).
- N. Lambert, Y.-N. Chen, Y.-C. Cheng, C.-M. Li, G.-Y. Chen, F. Nori, "Functional quantum biology in photosynthesis and magnetoreception", *arXiv:1205.0883v1* (2012). This work was reported in *News of Technology Review* published by MIT: "The Quantum Biology Conundrum" <http://www.technologyreview.com/blog/arxiv/27829/>

- N.S. Ginsberg, J.A. Davis, M. Ballottari, Y.-C. Cheng, R. Bassi, G.R. Fleming, “Solving structure in the CP29 light harvesting complex with polarization-phased 2D electronic spectroscopy”, *Proc. Nat. Acad. Sci. U.S.A.*, **108**, 3848 (2011).
- M. Sarovar, Y.-C. Cheng, K.B. Whaley, “Environmental correlation effects on excitation energy transfer in photosynthetic light harvesting”, *Phys. Rev. E*, **83**, 011906 (2011).
- T.C. Yen and Y.-C. Cheng, “Electronic coherence effects in photosynthetic light harvesting.”, In 22nd Solvay Conference on Chemistry, *Procedia Chemistry*, **3**, 211 (2011).
- G.R. Fleming, G.D. Scholes, and Y.-C. Cheng, “Quantum effects in biology.”, In 22nd Solvay Conference on Chemistry, *Procedia Chemistry*, **3**, 38 (2011).
- T. Calhoun, N. Ginsberg, G. Schlau-Cohen, Y.-C. Cheng, M. Ballottari, R. Bassi, G.R. Fleming, “Quantum Coherence Enabled Determination of the Energy Landscape in Light Harvesting Complex II.”, *J. Phys. Chem. B*, **113**, 16291 (2009).
- N.S. Ginsberg, Y.-C. Cheng, and G.R. Fleming, “Two-Dimensional Electronic Spectroscopy of Molecular Aggregates.”, *Acc. Chem. Res.*, **42**, 1352 (2009).
- Y.-C. Cheng and G.R. Fleming, “Dynamics of light harvesting in photosynthesis.”, *Ann. Rev. Phys. Chem.*, **60**, 241 (2009).
- S. Jang, Y.-C. Cheng, D.R. Reichman, and J.D. Eaves, “Theory of coherent resonance energy transfer.”, *J. Chem. Phys.*, **129**, 101104 (2008).
- Y.-C. Cheng, T.K. Ahn, T.J. Avenson, D. Zigmantas, K.K. Niyogi, M. Ballottari, R. Bassi, and G.R. Fleming, “Kinetic modeling of charge-transfer quenching in the CP29 minor complex.”, *J. Phys. Chem. B*, **112**, 13418 (2008).
- Y.-C. Cheng and R.J. Silbey, “A unified theory for charge-carrier transport in organic crystals.”, *J. Chem. Phys.*, **128**, 114713 (2008).
- T. Ahn, T.J. Avenson, M. Ballottari, Y.-C. Cheng, K.K. Niyogi, R. Bassi, G.R. Fleming, “Architecture of a charge-transfer state regulating light harvesting in a plant antenna protein.”, *Science*, **320**, 794 (2008).
- Y.-C. Cheng and G.R. Fleming, “Coherence quantum beats in two-dimensional electronic spectroscopy.”, *J. Phys. Chem. A*, **112**, 4254 (2008).
- H. Lee, Y.-C. Cheng, and G.R. Fleming, “Quantum coherence accelerating photosynthetic energy transfer.”, In *Ultrafast Phenomena XVI*, edited by P. Corkum, K. Nelson, E. Riedle, R. Schoenline, S. De Silvestri, (Springer, Berlin 2008).
- Y.-C. Cheng, G.S. Engel, and G.R. Fleming, “Elucidation of population and coherence dynamics using cross-peaks in two-dimensional electronic spectroscopy”, *Chem. Phys.*, **341**, 285 (2007).
- Y.-C. Cheng, H. Lee, and G.R. Fleming, “Efficient simulation of three-pulse photon-echo signals with application to the determination of electronic coupling in a bacterial photosynthetic reaction center.”, *J. Phys. Chem. A*, **111**, 9499 (2007).

- H. Lee, Y.-C. Cheng, and G.R. Fleming, “Coherence dynamics in photosynthesis: protein protection of excitonic coherence.”, *Science*, **316**, 1462 (2007).
- G.S. Engel, T.R. Calhoun, E.L. Read, T.K. Ahn, T. Mancal, Y.-C. Cheng, R.E. Blankenship, and G.R. Fleming, “Evidence for wavelike energy transfer through quantum coherence in photosynthetic systems.”, *Nature*, **446**, 782 (2007).
- Y.-C. Cheng and R.J. Silbey, “Coherence in the B800 ring of purple bacteria LH2.”, *Phys. Rev. Lett.*, **96**, 028103 (2006).
- Y.-C. Cheng and R.J. Silbey, “Markovian approximation in the relaxation of quantum open systems.”, *J. Phys. Chem. B*, **109**, 21399 (2005).
- Y.-C. Cheng and R.J. Silbey, “A microscopic quantum dynamics study on the noise threshold of fault-tolerant quantum error correction.”, *Phys. Rev. A*, **72**, 012320 (2005).
- Y.-C. Cheng and R.J. Silbey, “Stochastic Liouville equation approach for the effect of noise in quantum computations.”, *Phys. Rev. A*, **69**, 052325 (2004).
- E. Barkai and Y.-C. Cheng, “Aging continuous time random walks.”, *J. Chem. Phys.*, **118**, 6167 (2003).
- Y.-C. Cheng, R.J. Silbey, D.A. da Silva, J.P. Calbert, J. Cornil, and J.L. Bredas, “Three-dimensional band structure and bandlike mobility in oligoacene single crystals: a theoretical investigation.”, *J. Chem. Phys.*, **118**, 3764 (2003).
- Y.-C. Cheng, Y.K. Chen, T.M. Huang, C.I. Yu, G.H. Lee, Y. Wang, J.T. Chen, “Synthesis of metalla-cyclobutenes of late transition metals via nucleophilic addition of allenyl or propargyl complexes.”, *Organometallics*, **17**, 2953 (1998).