Jiri Vanicek

SCIENTIFIC ARTICLES WITH PEER REVIEW

[33] M. Wehrle, M. Sulc, and **J. Vanicek**: "On-the-fly ab initio semiclassical calculation of the time-resolved photoemission spectrum of azulene," in preparation (2012).

[32] M. Sulc, H. Hernandez Mendiola, T. J. Martinez, and **J. Vanicek**: "Gaussian dephasing representation: An exact semiclassically motivated method for quantum dynamics calculation of time-resolved electronic spectra," in preparation (2012).

[31] T. Zimmermann and **J. Vanicek**: "On-the-fly ab initio evaluation of the importance of spin-orbit couplings in nonadiabatic quantum dynamics," in preparation (2012).

[30] R. Marin and **J. Vanicek**: "Analysis of the accessibility of PAR-CLIP bound sites reveals that nucleation of the miRNA-mRNA pairing occurs at the 3' end of the seed match," submitted (2012).

[29] M. Sulc and **J. Vanicek**: "Accelerating the calculation of time-resolved electronic spectra with the cellular dephasing representation," *Molecular Physics* William H. Miller Festschrift, in press (2012).

[28] T. Zimmermann and **J. Vanicek**: "Measuring nonadiabaticity of molecular quantum dynamics with quantum fidelity and with its efficient semiclassical," *Journal of Chemical Physics* **136**, 094106 (2012).

[27] R. Marin and **J. Vanicek**: "Optimal use of conservation and accessibility filters in microRNA target prediction," *PLoS ONE* **7**, e32208 (2012).

[26] A. J. Olaya, D. H. Schaming, P.-F. M. Brevet, H. Nagatani, T. Zimmermann, **J. Vanicek**, H.-J. Xu, C. P. Gros, J.-M. Barbe and H. Girault, "Self-Assembled molecular rafts at liquid|liquid interfaces for four-electron oxygen reduction," *Journal of the American Chemical Society* **134**, 498 (2012).

[25] C. Mollica, T. Zimmermann, and **J. Vanicek**: "Efficient sampling avoids the exponential wall in classical simulations of fidelity," *Physical Review E* **84**, 066205 (2011).

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[22] M. Wehrle, M. Sulc, and **J. Vanicek**: "Accelerating calculations of ultrafast time-resolved electronic spectra with efficient quantum dynamics methods," *Chimia* **65**, 334 (2011).

[21] R. Marin and **J. Vanicek**: "Efficient use of accessibility in microRNA target prediction," *Nucleic Acids Research* **39**, 19 (2011).
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[20] K. Wong, J. Sonnenberg, F. Paesani, T. Yamamoto, **J. Vanicek**, W. Zhang, B. Schlegel, D. Case, T. Cheatham III, W. H. Miller, and G. Voth: "Proton Transfer Studied Using a Combined Ab Initio Reactive Potential Energy Surface with Quantum Path Integral Methodology," *Journal of Chemical Theory and Computation* **6**, 2566 (2010).

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BOOK CHAPTERS

[1] **J. Vanicek**: "Quantum instanton evaluation of the kinetic isotope effects and of the temperature dependence of the rate constant," in H. DaCosta, Ed., *Rate Constant Calculation for Thermal Reactions: Methods and Applications,* p. 67-92, John Wiley & Sons (2012).

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