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PUBLICATIONS

In International Peer Reviewed Journals:

1. Marius Buerkle, Umesha Perera, Florian Gimbert, Hisao Nakamura, Masaaki Kawata, and Yoshihiro Asai, "Deep-Learning Approach to First-Principles Transport Simulations", **Phys. Rev. Lett.** 126, 17701-1-4 (2021), DOI: 10.1103/PhysRevLett.126.177701.
2. Yueqi Li, Marius Buerkle, Guangfeng Li, Ali Rostamian, Hui Wang, Zixiao Wang, David R. Bowler, Tsuyoshi Miyazaki, Limin Xiang, Yoshihiro Asai, Gang Zhou & Nongjian Tao, "Gate controlling of quantum interference and direct observation of anti-resonances in single molecule charge transport", **Nature Materials**, 18, 357-363 (2019), DOI: 10.1038/s41563-018-0280-5.
3. Marius Buerkle, and Yoshihiro Asai, "How To Probe the Limits of the Wiedemann-Franz Law at Nanoscale", **Nano Lett.** 18, 7358-7361 (2018).
4. Hisao Nakamura, Ivan Rungger, Stefano Sanvito, Nobuki Inoue, Junji Tominaga and Yoshihiro Asai, "Resistive switching mechanism of GeTe-Sb₂Te₃ interfacial phase change memory and topological properties of embedded two-dimensional states", **Nanoscale**, 9, 9386-9395 (2017).
5. Marius Buerkle, Limin Xiang, Guangfeng Li, Ali Rostamian, Thomas Hines, Shaoyin Guo, Gang Zhou, Nongjian Tao, and Yoshihiro Asai, "The Orbital Selection Rule for Molecular Conductance as Manifested in Tetraphenyl-Based Molecular Junctions", **J. Am. Chem. Soc.** 139, 2989-2993 (2017).
6. Marius Buerkle and Yoshihiro Asai, **Sci. Rep.** 7, 41898-1-7 (2017).
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8. Hisao Nakamura and Yoshihiro Asai, "Competitive effects of oxygen vacancy formation and interfacial oxidation on an ultra-thin HfO₂-based resistive switching memory: beyond filament and charge hopping models", **Phys. Chem. Chem. Phys.** 18, 8820-8826 (2016).
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10. See Kei Lee, Marius Buerkle, Ryo Yamada, Yoshihiro Asai and Hirokazu Tada, "Thermoelectricity at the molecular scale: a large Seebeck effect in endohedral metallofullerenes", **Nanoscale**, 7, 20497-20502 (2015).
11. Delia Miguel, Luis Álvarez de Cienfuegos, Ana Martín-Lasanta, Sara P. Morcillo, Linda A. Zotti, Edmund Leary, Marius Buerkle, Yoshihiro Asai, Rocío Jurado, Diego J. Cárdenas, Gabino Rubio-Bollinger, Nicolás Agraït, Juan M. Cuerva, and M. Teresa González, "Towards multiple conductance pathways with heterocycle-based oligo (phenyleneethynylene) derivatives", **J. Am. Chem. Soc.** 137, 13818-13826 (2015).
12. Raúl García, M. Ángeles Herranz, Edmund Leary, M. Teresa González, Gabino Rubio Bollinger, Marius Buerkle, Linda A. Zotti, Yoshihiro Asai, Fabian Pauly, Juan Carlos Cuevas, Nicolás Agraït and Nazario Martín, "Single-molecule conductance of a chemically modified, π -extended tetrathiafulvalene and its charge-transfer complex with F4TCNQ", **Beilstein J. Org. Chem.** 11, 1068-1078 (2015).
13. Marius Buerkle, Thomas J. Hellmuth, Fabian Pauly, and Yoshihiro Asai, "First-principles calculation of the thermoelectric figure of merit for [2,2] paracyclophane-based single-molecule junctions", **Phys. Rev. B**, 91, 165419-1-8 (2015).
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15. L.A. Zotti, M. Buerkle, F. Pauly, W. Lee, K. Kim, W. Jeong, Y. Asai, P. Reddy and J.C. Cuevas, "Heat dissipation and its relation to thermopower in single-molecule junctions", **New J. Phys.** 16, 015004-1-25 (2014).
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- Formation of Single-Molecule Junctions by Electrochemical Reduction of Diazonium Terminal Groups”, **J. Am. Chem. Soc.** 135, 3319–3322 (2013): **Communication**.
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 20. See Kei Lee, Ryo Yamada, Shoji Tanaka, Gap Soo Chang, Yoshihiro Asai, and Hirokazu Tada, “Universal Temperature Crossover Behavior of Electrical Conductance in a Single Oligothiophene Molecular Wire”, **ACS Nano**, 6, 5078-5082 (2012).
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