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First Principles Charge Transfer Excitations in Curved Aromatic Materials LAURA ZOPPI, University of Zurich, LAYLA MARTIN SAMOS, University of Nova Gorica, KIM K. BALDRIDGE, University of Zurich — Understanding excitation properties and charge transport phenomena of curved π-conjugated materials is critical for a rational utilization of buckybowls as electrically active materials in solid-state devices. In this respect, the class of materials based on the smallest bowl-shaped fullerene fragment, corannulene, $C_{20}H_{10}$, offers a unique possibility for building up scaffolds with a tunable spectrum of structural and electronic properties.[1] Here, GW-BSE based approaches are applied to investigation and prediction of charge transfer excitations of $C_{20}H_{10}$ materials systems at functional interfaces, [1-3] with a special emphasis on design aspects of materials relevant in the experimental domain. Theoretical predictions together with experimental findings illustrate the possibility of integrating corannulene electronic functions in molecular devices. [1] L. Zoppi, L. Martin-Samos, K. K. Baldridge, *Acc. Chem. Res.*, 47, 3310–3320 (2014) [2] L. Zoppi, L. Martin-Samos, K. K. Baldridge*, J. Am. Chem. Soc.* 133, 14002-14009 (2011) [3] L. Zoppi, L. Martin Samos, K. K. Baldridge, *Phys. Chem. Chem. Phys.* 17, 6114-6121 (2015)

Laura Zoppi
University of Zurich

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