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J. Chem. Phys. **142**, 124113 (2015); http://dx.doi.org/10.1063/1.4916390

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J. Chem. Phys. **142**, 124302 (2015); http://dx.doi.org/10.1063/1.4916035

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Chengyin Wu, Cong Wu, Yameng Fan, Xiguo Xie, Peng Wang, Yongkai Deng, Yunquan Liu and Qihuang Gong
J. Chem. Phys. **142**, 124303 (2015); http://dx.doi.org/10.1063/1.4916045

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J. Chem. Phys. **142**, 124304 (2015); http://dx.doi.org/10.1063/1.4915142

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J. Chem. Phys. **142**, 124307 (2015); http://dx.doi.org/10.1063/1.4915889

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J. Chem. Phys. **142**, 124309 (2015); http://dx.doi.org/10.1063/1.4916122

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Errata

Erratum: “Electronic couplings for molecular charge transfer: Benchmarking CDFT, FODFT, and FODFTB against high-level ab initio calculations” [J. Chem. Phys. 140, 104105 (2014)]

Adam Kubas, Felix Hoffmann, Alexander Heck, Harald Oberhofer, Marcus Elstner andJochen Blumberger

J. Chem. Phys. **142**, 129905 (2015); http://dx.doi.org/10.1063/1.4916382