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A hybrid version of the SCAN functional including long-range dispersion interactions¹ HSIN-YU KO, MARCOS F. CALEGARI ANDRADE, BISWAJIT SANTRA, ANNABELLA SELLONI, ROBERTO CAR, Princeton University — The recently developed meta-GGA density functional, called SCAN (strongly constrained and appropriately normed) [1], provides an accurate description of the electronic structure in a broad class of systems characterized by different bonding interactions, including intermediate range van-der-Waals (vdW) bonding [2]. Here we consider a hybrid version of the SCAN functional [3] with inclusion of long-range vdW interactions via a re-parameterized Tkatchenko-Scheffler scheme [4]. Calculations for the S22 molecular database, ice hexamer clusters, and bulk ice Ih indicate that this functional further improves the description of vdW and hydrogen bonding interactions. [1] J Sun, A Ruzsinszky, and J P Perdew, PRL 115, 036402 [2] J Sun et al, Nat Chem 8, 831 [3] K Hui and J-D Chai, JCP 144, 044114 [4] A Tkatchenko and M Scheffler, PRL 102, 073005

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