

Abstract Submitted  
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**Application of van der Waals Density Functionals to Extended Systems**<sup>1</sup> KYUHO LEE, DAVID C. LANGRETH, Rutgers University — Recently we proposed<sup>2</sup> a second version of a van der Waals density functional<sup>3</sup> and showed its accuracy for small molecular duplexes as well as a few extended systems. As further applications to extended systems, we present results for molecular adsorptions on surfaces, molecular crystals, and organic ferroelectrics. A comparison with experiments is also given for different functionals.

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<sup>2</sup>K. Lee, É. D. Murray, L. Kong, B. I. Lundqvist, and D. C. Langreth, Phys. Rev. B **82**, 081101(R) (2010).

<sup>3</sup>M. Dion, H. Rydberg, E. Schröder, D. C. Langreth, and B. I. Lundqvist, Phys. Rev. Lett. **92**, 246401 (2004); T. Thonhauser, V. R. Cooper, S. Li, A. Puzder, P. Hyldgaard, and D. C. Langreth, Phys. Rev. B **76**, 125112 (2007).

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