Application of van der Waals Density Functionals to Extended Systems\textsuperscript{1} KYUHO LEE, DAVID C. LANGRETH, Rutgers University — Recently we proposed\textsuperscript{2} a second version of a van der Waals density functional\textsuperscript{3} 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.

\textsuperscript{1}Work supported by NSF grant DMR-0801343.


Kyuho Lee
Rutgers University

Date submitted: 16 Nov 2010