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Subsystem functional for confinement physics FENG HAO, ANN MATTSSON, Sandia National Laboratories, RICKARD ARMIENTO, MIT — Recent success of the AM05 [1,2] functional shows that the subsystem functional scheme is a practical framework to construct well-performing functionals in density functional theory (DFT). The idea is to divide the real material system into regions with different characteristic physics that can be described by model systems. In AM05, subsystem functionals based on a surface model system and a uniform electron gas model system are combined to include both the edge and interior physics. By studying a harmonic oscillator model system restricted in one dimension, we are aiming to build a subsystem functional that can include "confinement physics" into the scheme. The new model system may help in constructing a more generally accurate functional working for both solid-state and chemical systems. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. [1] R. Armiento, A.E. Mattsson, PRB 72, 085108 (2005), [2] A.E. Mattsson et al. JCP 128, 084714 (2008).

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