Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

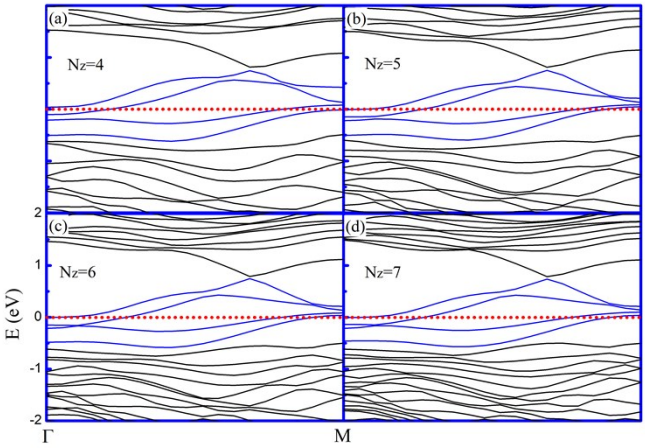

Figure S1. *Calculated band structure for the zigzag MoSSe nanoribbons as a function of its width as measured by the Nz parameter. (a) Nz=4, (b) Nz=5, (c) Nz=6, (d) Nz=7. The horizontal dotted red line marks the Fermi level, set as energy reference (0 eV).*

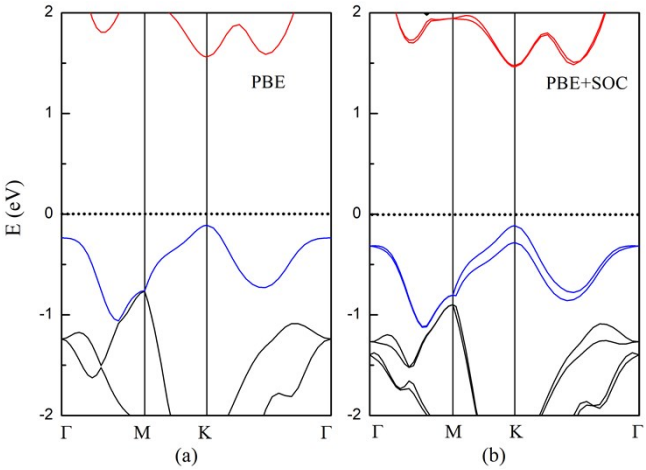

Figure S2. *Calculated band structure of the two-dimensional MoSSe sheet at the (a) PBE and (b) PBE+SOC level. The horizontal black dotted line marks the Fermi level, set at 0 eV.*

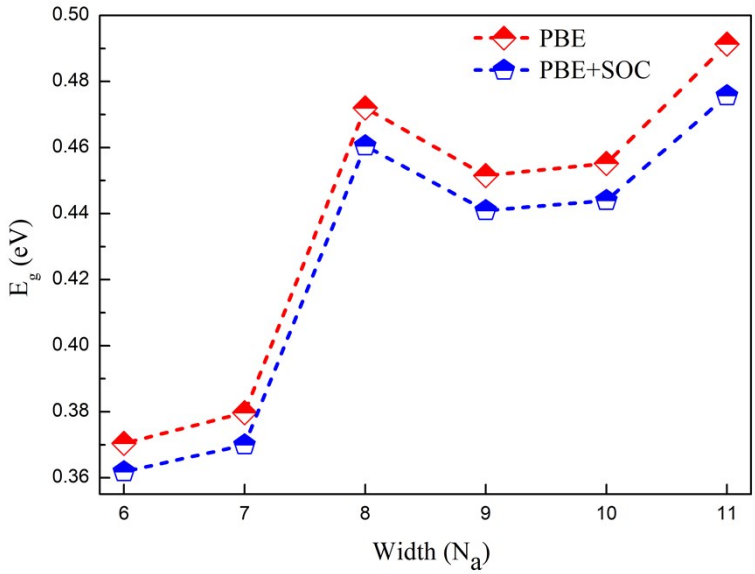

Figure S3. *Calculated band gap for the armchair MoSSe nanoribbons as a function of its width as denoted by the N_a parameter in the 6 to 11 range. The red dotted line has been calculated at the PBE level, and the blue dotted line at the PBE+SOC level.*

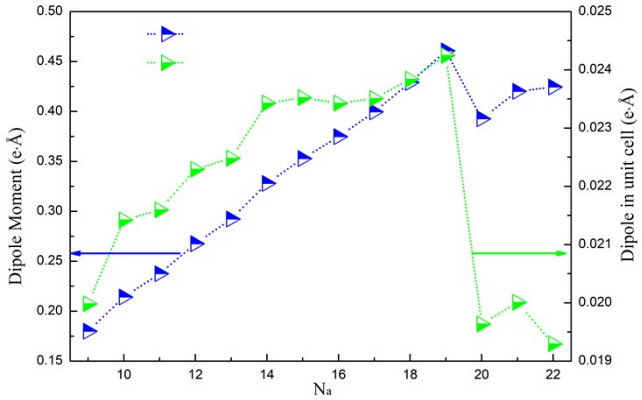

Figure S4*. Calculated dipole moment for the zigzag MoSSe nanoribbons as a function of its width as measured by the N_a parameter in the 9 to 22 range. The right vertical axis reports the dipole moment per unit cell of the nanoribbon.*

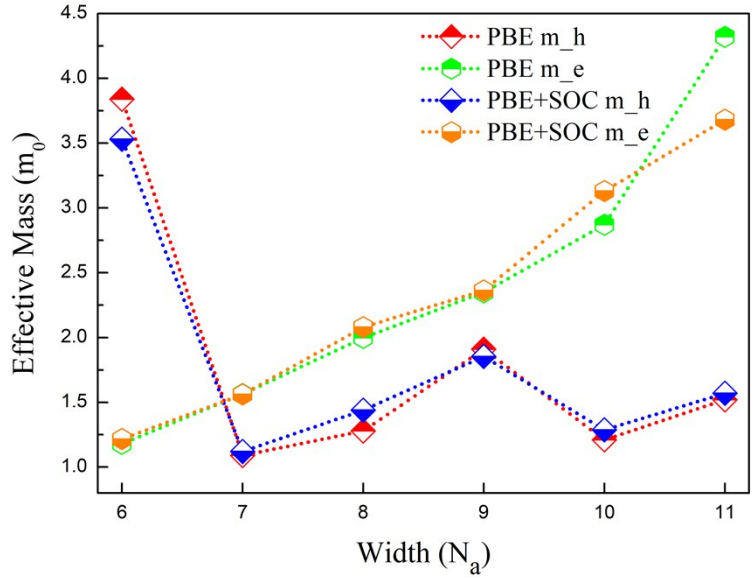

Figure S5. *Calculated effective mass of electron and hole for the armchair MoSSe nanoribbons as a function of its width as measured by the N_a parameter. The red and green dotted traces report the PBE hole and electron mass, respectively. The blue and orange dotted traces show the PBE+SOC hole and electron mass, respectively.*

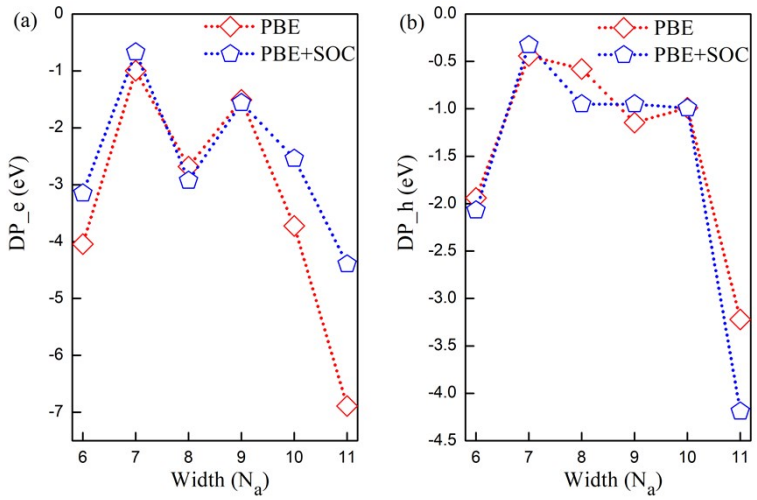

Figure S6. *Calculated deformation potential (DP) of (a) electron and (b) hole for the armchair MoSSe nanoribbons as a function of its width as measured by the N_a parameter. Red and blue symbols report the PBE and PBE+SOC results, respectively.*

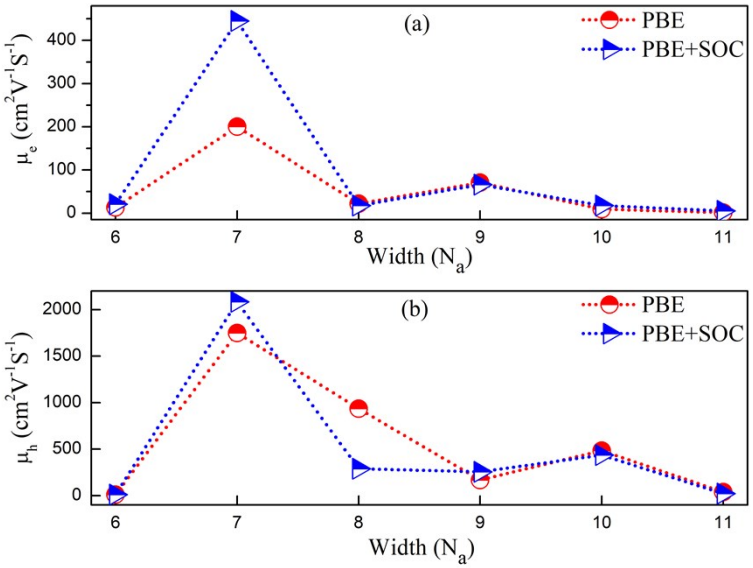

Figure S7. *Calculated carrier mobility of (a) electron and (b) hole for the armchair MoSSe nanoribbons as a function of its width as measured by the N_a parameter. Red and blue symbols report the PBE and PBE+SOC results, respectively.*