

## Supporting Information

### Theoretical study of p-n homojunction SiGe field-effect transistor *via* covalent functionalization

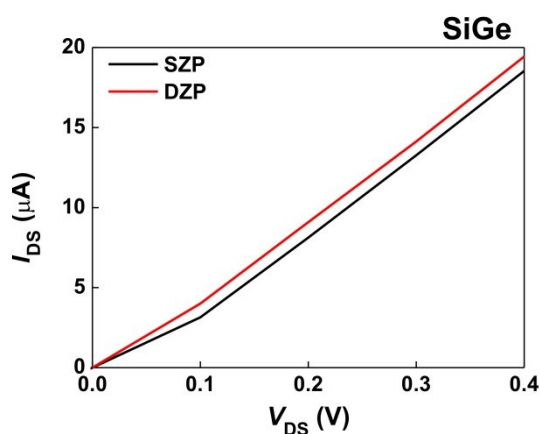
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**Figure S1.** Output characteristic of pristine SiGe FET at  $V_G = 0$  V with single- $\zeta$ -polarized (SZP) and double- $\zeta$ -polarized (DZP) basis sets, respectively.