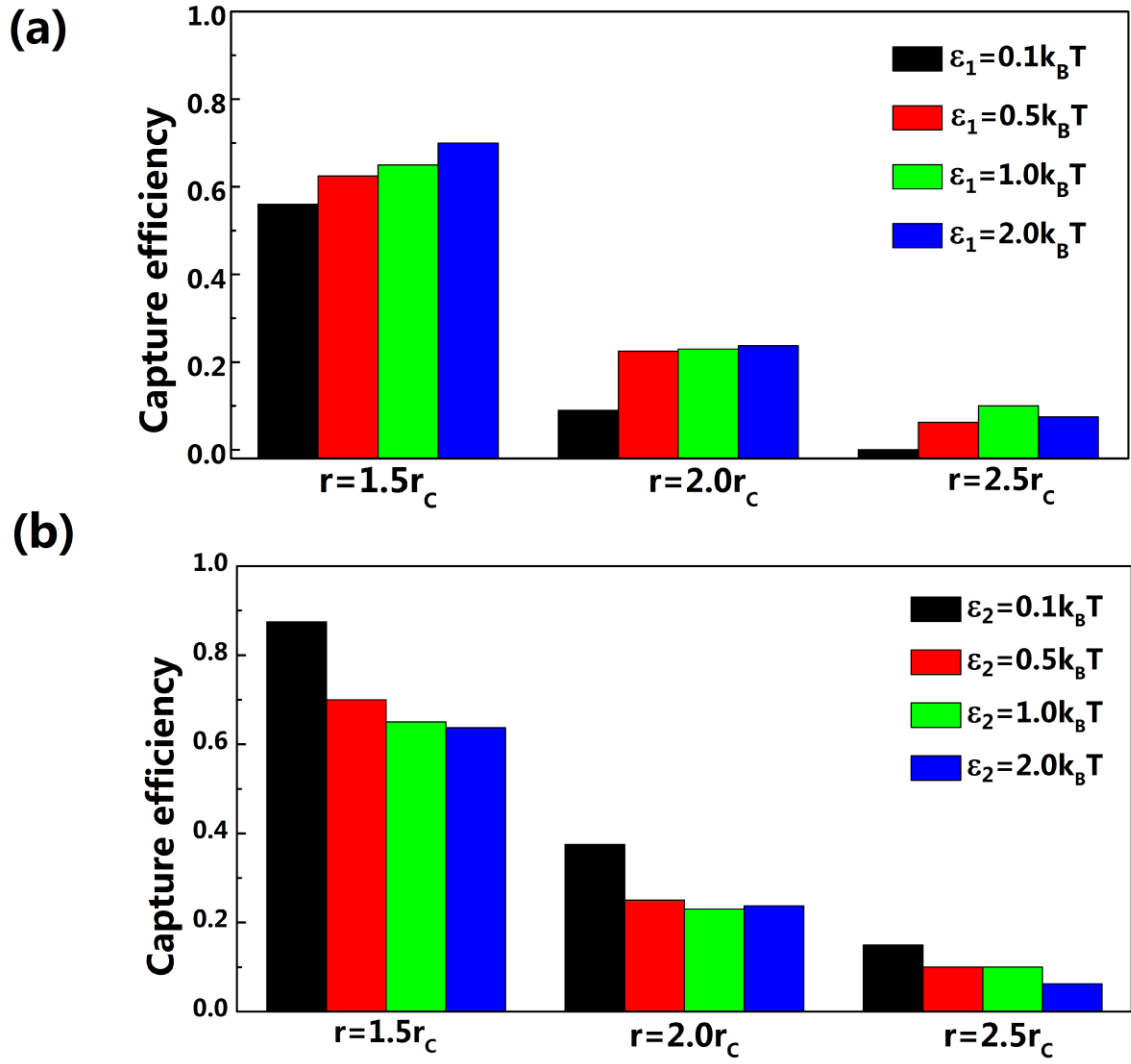**Supporting Information**

Computational design of functionalized substrate for capturing nanoparticles with specific size and shape
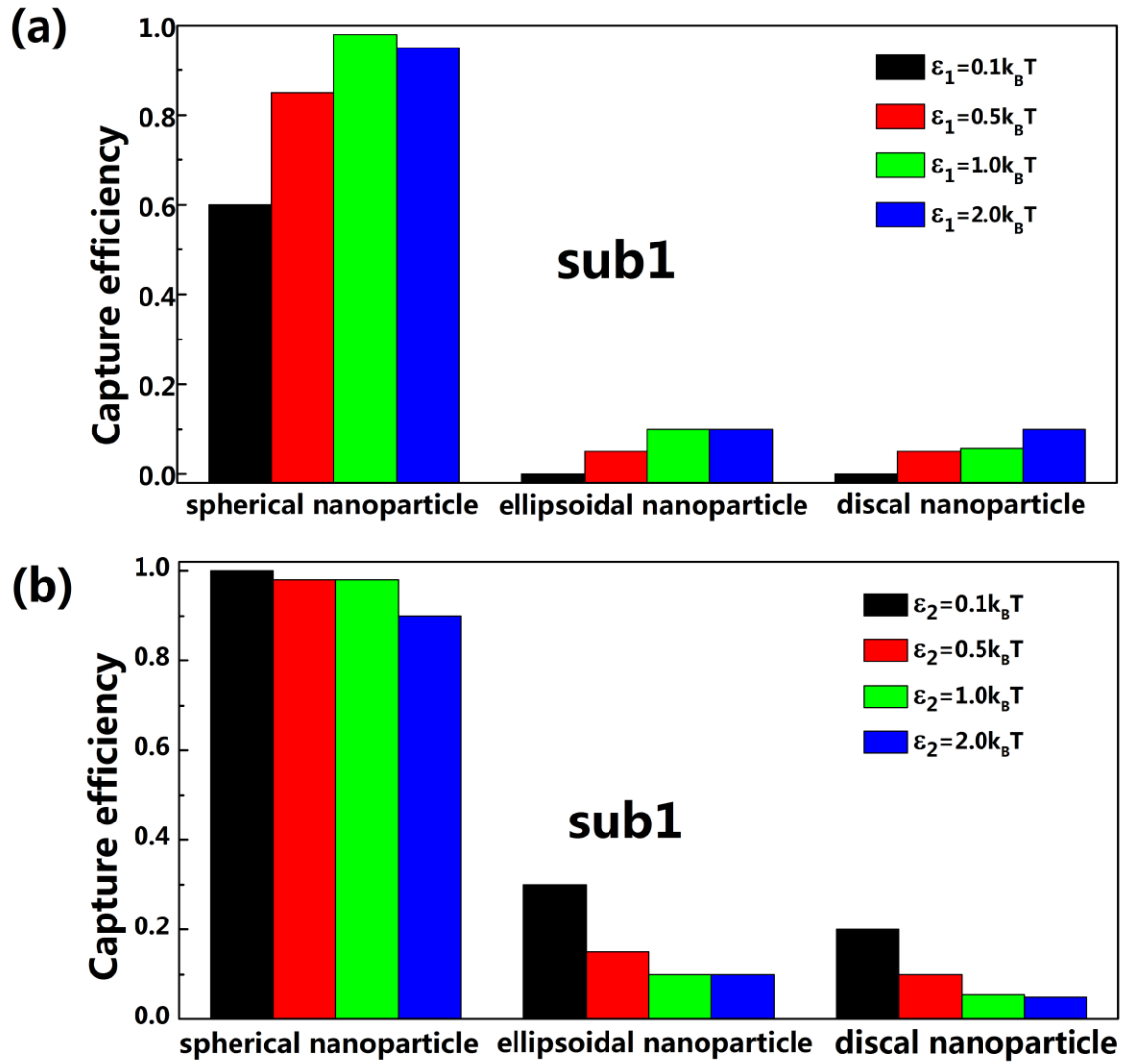
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Figure S1. The capture efficiency of spherical nanoparticles as a function of the nanoparticle size under different interaction parameters. (a) The strength of the attractive interaction (ε_1) between the nanoparticle and the specific part of copolymers changes from 0.1 k_BT to 2.0 k_BT, where the strength of the repulsive interaction (ε_2) between the nanoparticle and the non-specific part of copolymers is fixed as 1.0 k_BT. (b) The repulsive interaction (ε_2) changes from 0.1 k_BT to 2.0 k_BT, where the strength of attractive interaction (ε_1) is fixed as 1.0 k_BT.

Figure S2. The capture efficiency of nanoparticles with different shapes under different interaction parameters when the hole in the substrate is sphere. (a) The strength of the attractive interaction (ε_1) between the nanoparticle and the specific part of copolymers changes from 0.1 k_BT to 2.0 k_BT, where the strength of the repulsive interaction (ε_2) between the nanoparticle and the non-specific part of copolymers is fixed as 1.0 k_BT. (b) The repulsive interaction (ε_2) changes from 0.1 k_BT to 2.0 k_BT, where the strength of attractive interaction (ε_1) is fixed as 1.0 k_BT.