**Supporting materials**

**Details on models**

The two essential factors are discussed, i.e., the diameters of CNTs, the depth of water clusters, and the temperature of the system is set as 300 K. The diameters of nanocapsule and CNTs are labeled as *d*capsule and *d*CNT. The numbers of carbon atoms on the CNTs, nanocapsule and graphene pedestal are labeled as *N*CNT, *N*capsule and *N*pedestal, respectively. *N*water for water molecules in the CNTs. The parameters of the models in simulation are listed in the following tables.

Table S1: Parameters of the four models in simulations.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Model | 0.4d-CNT | 0.6d-CNT | 0.8d-CNT | 1.0d-CNT |
| CNT Chirality | (20, 20) | (30, 30) | (40, 40) | (50, 50) |
| Capsule Chirality | (15, 15) | (25, 25) | (35, 35) | (45, 45) |
| MD Box Size (Å3) | 500 × 500 × 1250 | 500 × 500 × 1250 | 500 × 500 × 1250 | 500 × 500 × 1250 |
| *d*capsule (Å) | 20.3 | 33.9 | 47.5 | 61.0 |
| *D*CNT (Å) | 27.1 | 40.7 | 54.2 | 67.8 |
| *N*water | 824 | 2131 | 3252 | 5716 |
| *N*CNT | 4000 | 6000 | 8000 | 10000 |
| *N*capsule | 642 | 1342 | 2262 | 3423 |
| *N*pedestal | 7868 | 7868 | 7868 | 7868 |

Table S2: Parameters of the 0.6d-CNT model with different depths of water clusters.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Model | *H* = 50 Å | *H* = 60 Å | *H* = 70 Å | *H* = 80 Å |
| CNT Chirality | (30, 30) | (30, 30) | (30, 30) | (30, 30) |
| Capsule Chirality | (25, 25) | (25, 25) | (25, 25) | (25, 25) |
| MD Box Size (Å3) | 500 × 500 × 1250 | 500 × 500 × 1250 | 500 × 500 × 1250 | 500 × 500 × 1250 |
| *d*capsule (Å) | 33.90 | 33.90 | 33.90 | 33.90 |
| *D*CNT (Å) | 40.68 | 40.68 | 40.68 | 40.68 |
| *N*water | 1536 | 1841 | 2131 | 2423 |
| *N*CNT | 6000 | 6000 | 6000 | 6000 |
| *N*capsule | 1342 | 1342 | 1342 | 1342 |
| *N*pedestal | 7868 | 7868 | 7868 | 7868 |

**The values of *v*out for the capsules in four models**

Table S3: The values of *v*out of the capsules in different CNTs when *E* is near the *E*CMax at 300 K.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 0.4d-CNT | ***E* (V/Å)** | **8.1** | **8.2** | **8.3** | **8.4** | **8.5** | **8.6** |
| *v*out (Å/ps) | 6.46 | 6.60 | 6.92 | 7.11 | 7.11 | 7.10 |
| 0.6d-CNT | ***E* (V/Å)** | **5.1** | **5.2** | **5.3** | **5.4** | **5.5** | **5.6** |
| *v*out (Å/ps) | 5.63 | 5.65 | 5.66 | 5.67 | 5.69 | 5.72 |
| 0.8d-CNT | ***E* (V/Å)** | **4.1** | **4.2** | **4.3** | **4.4** | **4.5** | **4.6** |
| *v*out (Å/ps) | 5.28 | 5.25 | 5.29 | 5.36 | 5.38 | 5.41 |
| 1.0d-CNT | ***E* (V/Å)** | **4.1** | **4.2** | **4.3** | **4.4** | **4.5** | **4.6** |
| *v*out (Å/ps) | 5.11 | 5.17 | 5.19 | 5.22 | 5.20 | 5.21 |

**Supplementary figures**

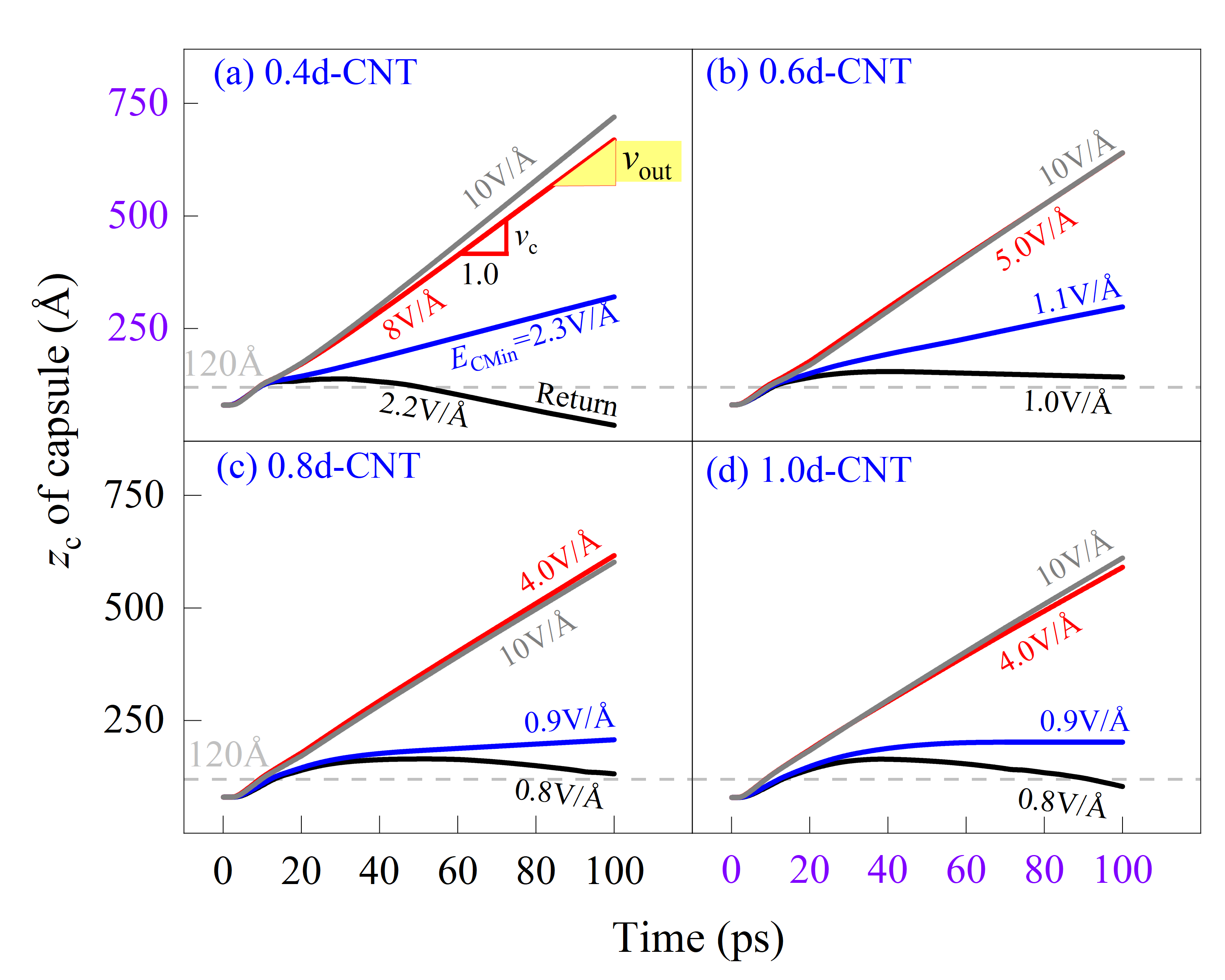


Figure S1: Evolution of the mass center and the exit velocity (vout) of the capsule in the z-/axial direction at 300 K when sinking in the EF with E ≤ 10 V/Å lasting 20 ps. The water depths are the same, i.e., H = 70 Å. Mass center in (a) 0.4d-CNT, (b) 0.6d-CNT, (c) 0.8d-CNT, or (d) 1.0d-CNT.

We discuss the effect of CNT size on the exit velocity (*v*out) of the capsule, which corresponds to the slope of the curve shown in Figure S1, particularly the red curve in Figure S1a. The *v*out of the capsule is calculated as mean value of *v*c over the interval of [80, 100] ps. In Figure S1a, the curves corresponding to *E* ≥ 2.3 V/Å exhibit positive slopes indicating that the capsule can escape from the CNT. Conversely, when *E* = 2.2 V/Å, the curve displays a negative slope after approximately 40 ps illustrating that the capsule returns to the CNT, signifying a failure to escape. Thus, the critical minimum electric field intensity (labeled as *E*CMin) required for the capsule to escape from the 0.4d-CNT is 2.3 V/Å. Notably, *E*CMin decreases with increasing CNT diameter; for example, *E*CMin is 1.1 V/Å for the 0.6d-CNT model and 0.9 V/Å for the 0.8d-CNT and1.0d-CNT models.

The results presented in Figure S1a-d indicate that as the electric field intensity (*E*) approaches 10 V/Å, the slope of the *z*c-curve changes only slightly. This suggests the existence of a maximum electric field intensity (labeled as *E*CMax) that can efficiently increase the value of *v*out within a given CNT.

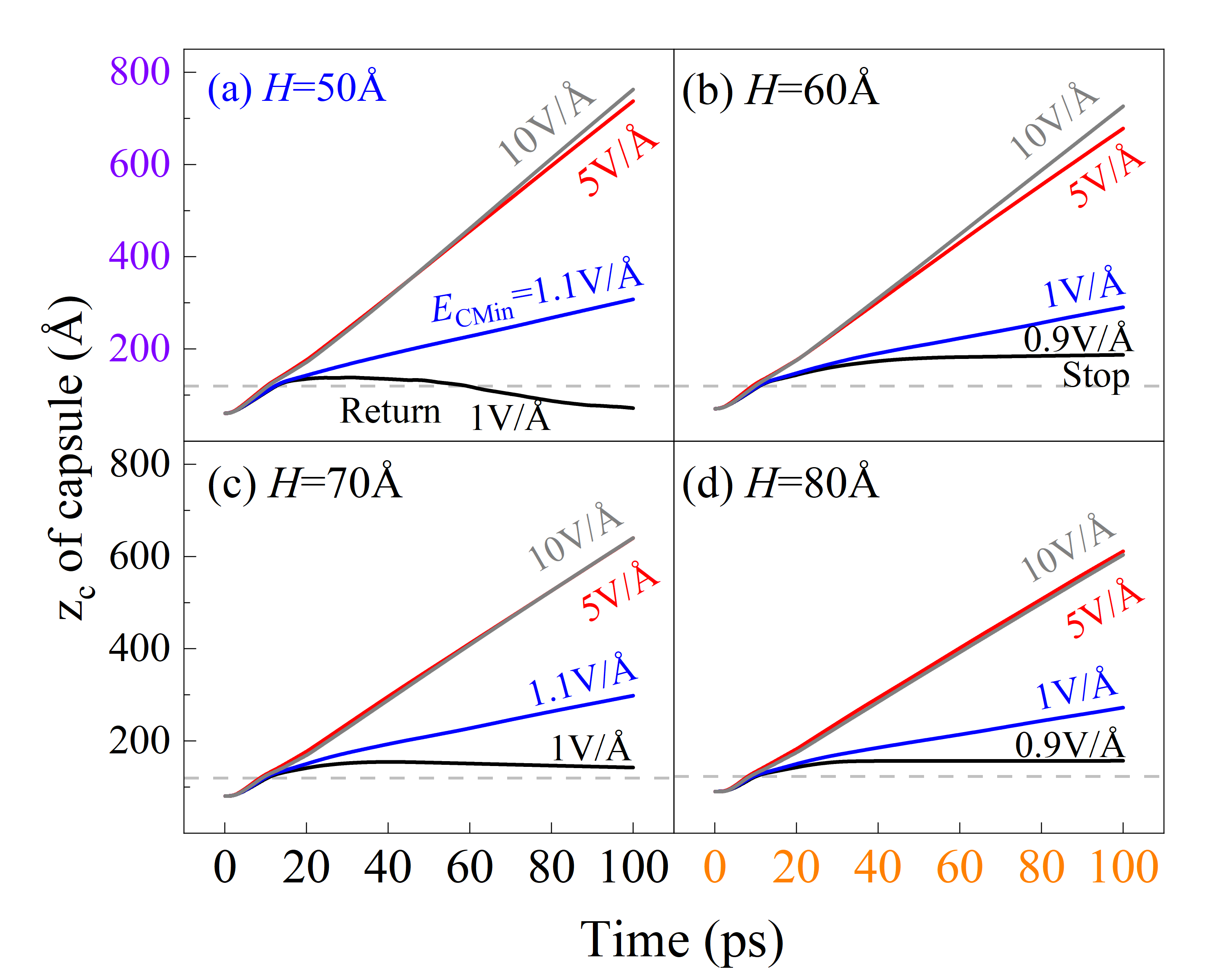


Figure S2: Motions of the mass center of the capsule in the z-/axial direction at 300 K when sinking in the EF with *E* ≤ 10 V/Å lasting 20 ps. The water depths are the different, i.e., (a) *H*=50 Å, (b) 60 Å, (c) 70 Å, or (d) 80 Å.

We calculated the values of *E*CMin, which represents the minimal EF intensity required to eject the capsule from the CNT, when the EF is applied for a fixed duration (e.g., *s* = 20 ps). As the water depth (*H*) increases from 50 Å to 80 Å, the corresponding *E*CMin values are 1.1 V/Å, 1.0 V/Å, 1.1 V/Å, and 1.0 V/Å, respectively (Figure S2). This indicates that variations in water depth *H* within the same CNT have no significant effect on *E*CMin. The underlying mechanism is that in a CNT with fixed geometry and physical properties, water depth only affects the number of water molecules. When subjected to the same critical EF, the axial expansion speed of the water cluster remains constant, providing the same impulse to the capsule. This allows the capsule to overcome the same attraction from the CNT, provided that the CNT is sufficiently long for the water cluster to fully expand.

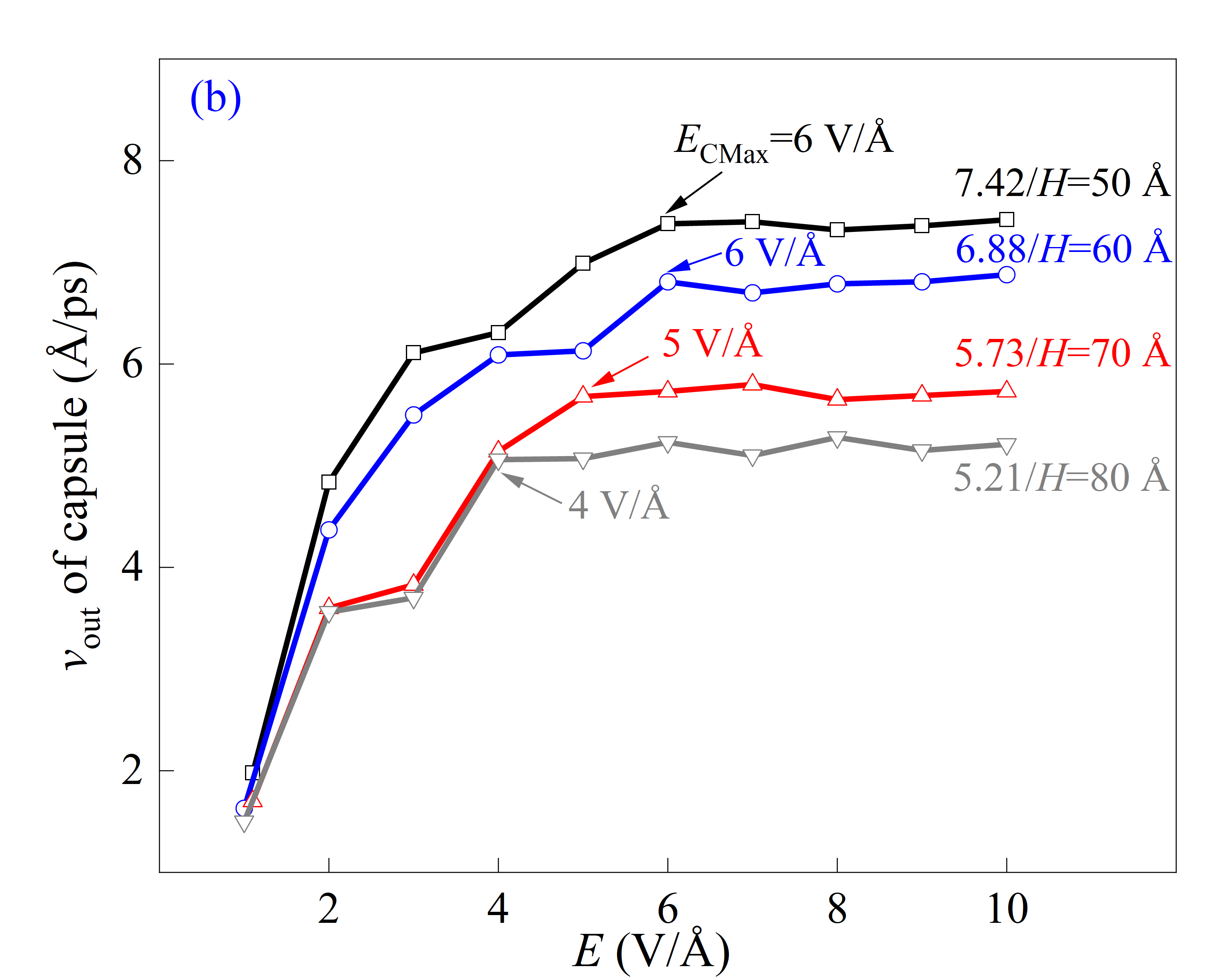
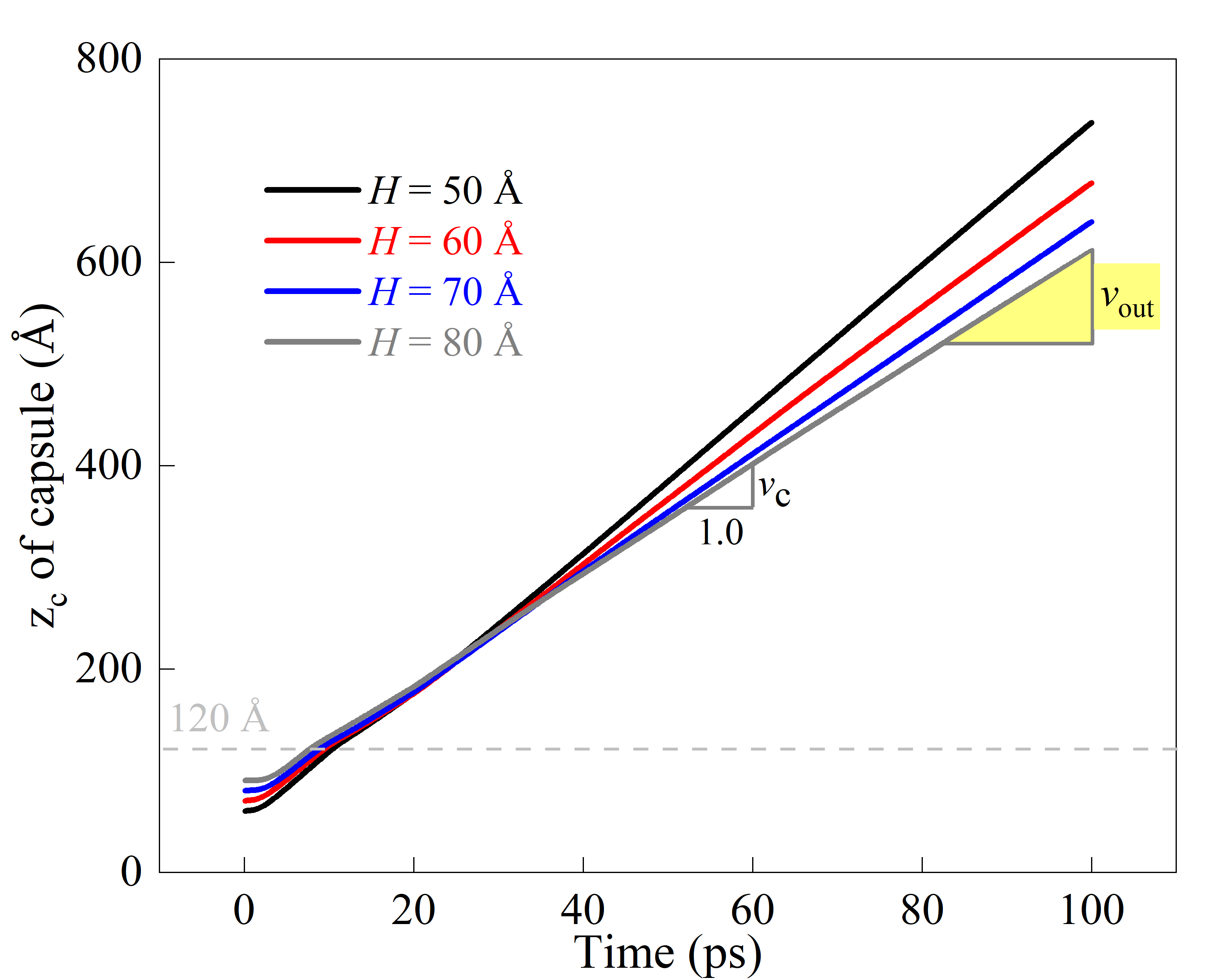


Figure S3: Responses of the capsule in the 0.6d-CNT model. (a) Evolution of the axial mass center of the capsule in the CNT with different water depths at 300 K when sinking in the same EF with *E* = 5 V/Å and *s* = 20 ps. The exit velocity (*v*out) of the capsule is the mean value of *v*c evaluated between 80 ps and 100 ps. (b) *v*out of the capsule versus the EF intensity.

Figure S3 shows the evolution of the mass center of the capsule when sinking in the EF with *E* = 5 V/Å and *s* = 20 ps. A decrease in water depth results in an increased *v*out. For example, *v*out = 6.99 Å/ps when *H* = 50 Å, *v*out = 6.13 Å/ps when *H* = 60 Å, *v*out = 5.68 Å/ps when *H* = 70 Å, and *v*out = 5.07 Å/ps when *H* = 80 Å. The mechanism is that, when *H* is lower, the distance between the capsule and the open end of the same CNT is greater. Consequently, the acceleration pathway and duration for the capsule are extended, allowing the capsule to achieve a higher value of *v*out.

We also calculated the values of *E*CMax for the same CNT varying water depths *H*. Based on the value of *v*out under different EF intensities, as shown in Figure S3b, when *H* ≤ 60 Å, the value of *v*out continues to increase as the EF intensity increases, up to a threshold of 6 V/Å. Beyond this point, *v*out converges, indicating that *E*CMax =~ 6 V/Å. For the model with *H* = 70 Å, *E*CMax =~ 5 V/Å, and *E*CMax =~ 4 V/Å for *H* = 80 Å, respectively. Thus, in the 0.6d-CNT model, as the water depth increases, both *v*out and the corresponding *E*CMax decreases.