Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Supporting Information

Rectification direction inversion in a phosphododecamolybdic acid / single-walled carbon nanotube junction

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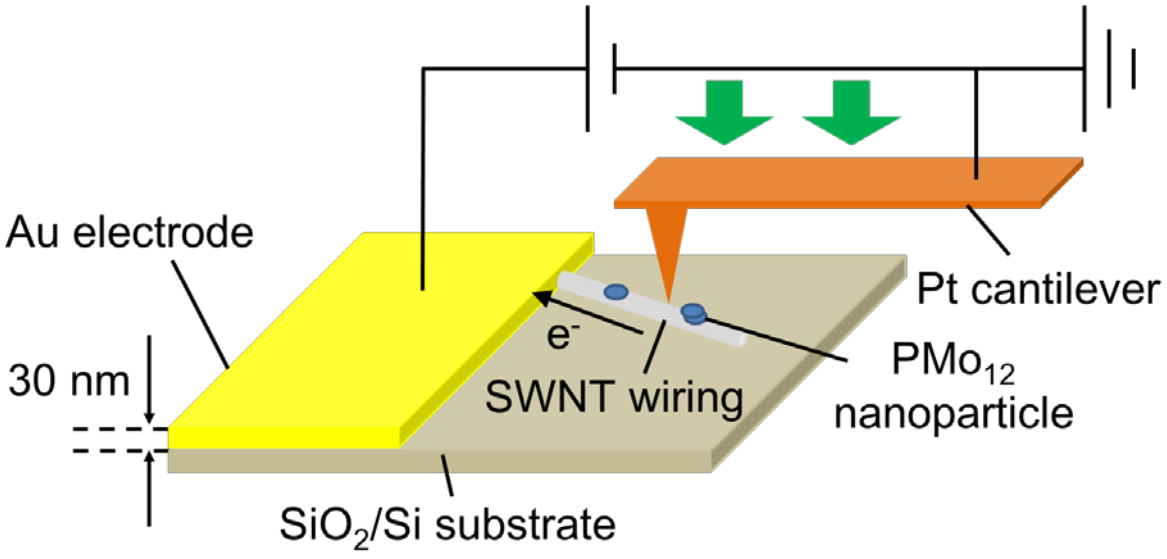

Figure S1. Experimental setup for measurement of the electronic properties of PMo_{12} adsorbed on SWNT using PCI-AFM. Detailed procedure of PCI-AFM measurement can be found in the literatures published previously.[1-3]

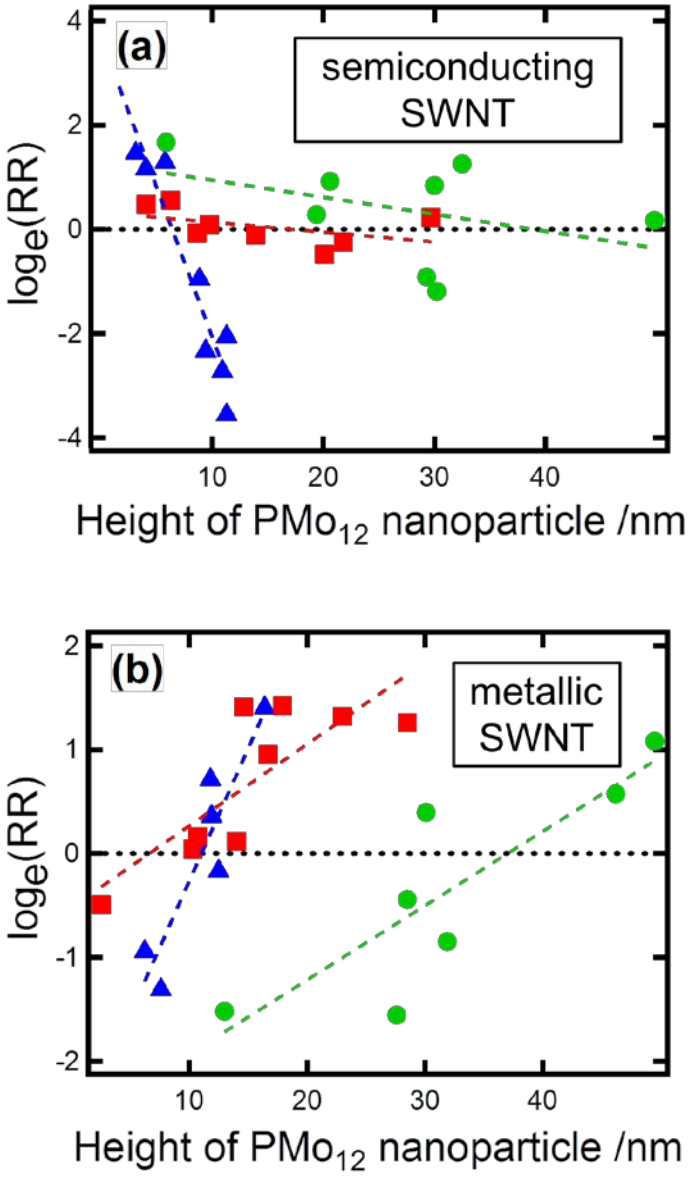

Figure S2. Plots of $\log_e$(RR) observed by PCI-AFM vs. PMo_{12} nanoparticle height for (a) PMo_{12}/semiconducting SWNT complex and (b) PMo_{12}/metallic SWNT complex. Each graph is obtained from *I-V* data of three individual PMo_{12}/SWNT complexes, which are indicated by red square, blue triangle and green circle respectively. Dashed lines are used just as guides to the eye. As the PMo_{12} nanoparticle size increases, $\log_e$(RR) decreases in the case of semiconducting SWNT, while increases for metallic SWNT, therefore the reproducibility of the results of rectification direction inversion is confirmed.

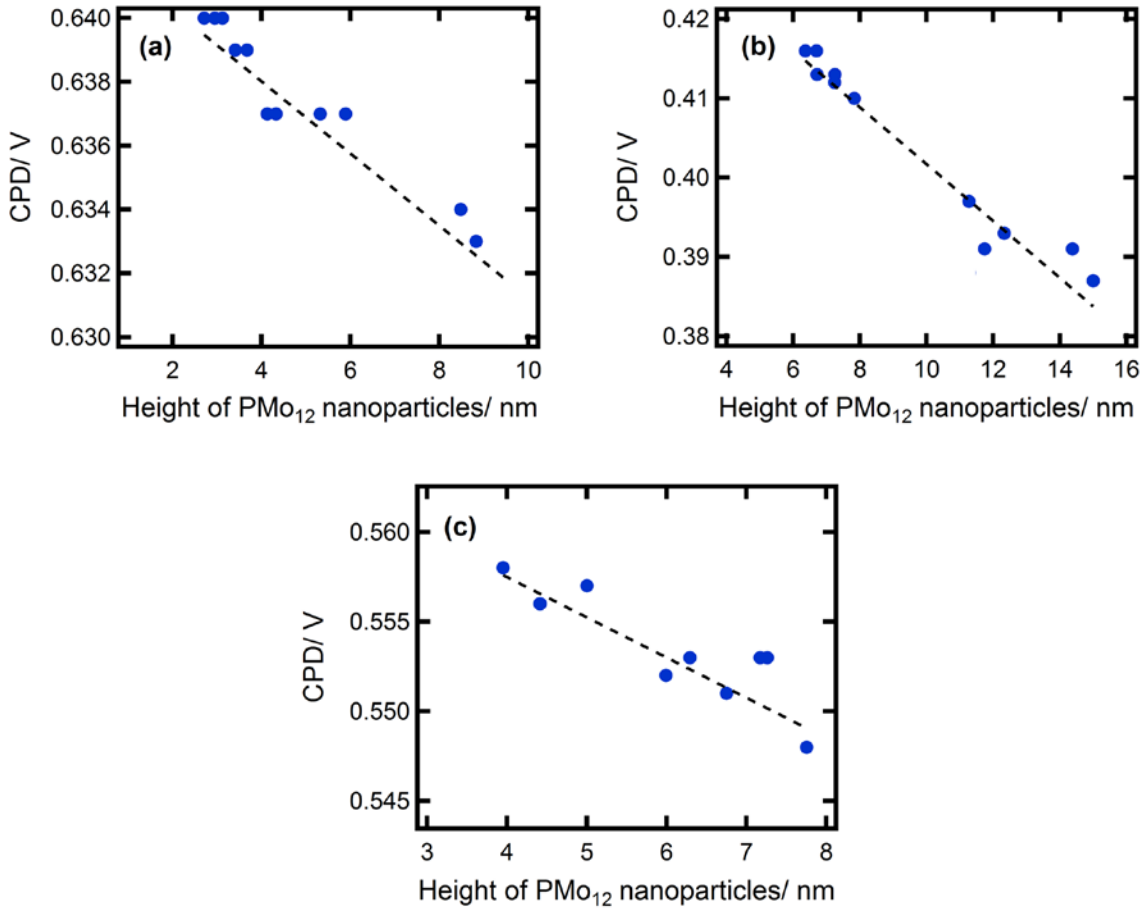

Figure S3. Plots of CPD value against complex height of PMo_{12}/semiconducting SWNT for three individual complexes. Dashed lines are used just as guides to the eye. In all the three plots, CPD value decreases as complex height increases. Therefore, the reproducibility of the relationship between CPD value and height of PMo_{12} particle on semiconducting SWNT is confirmed.

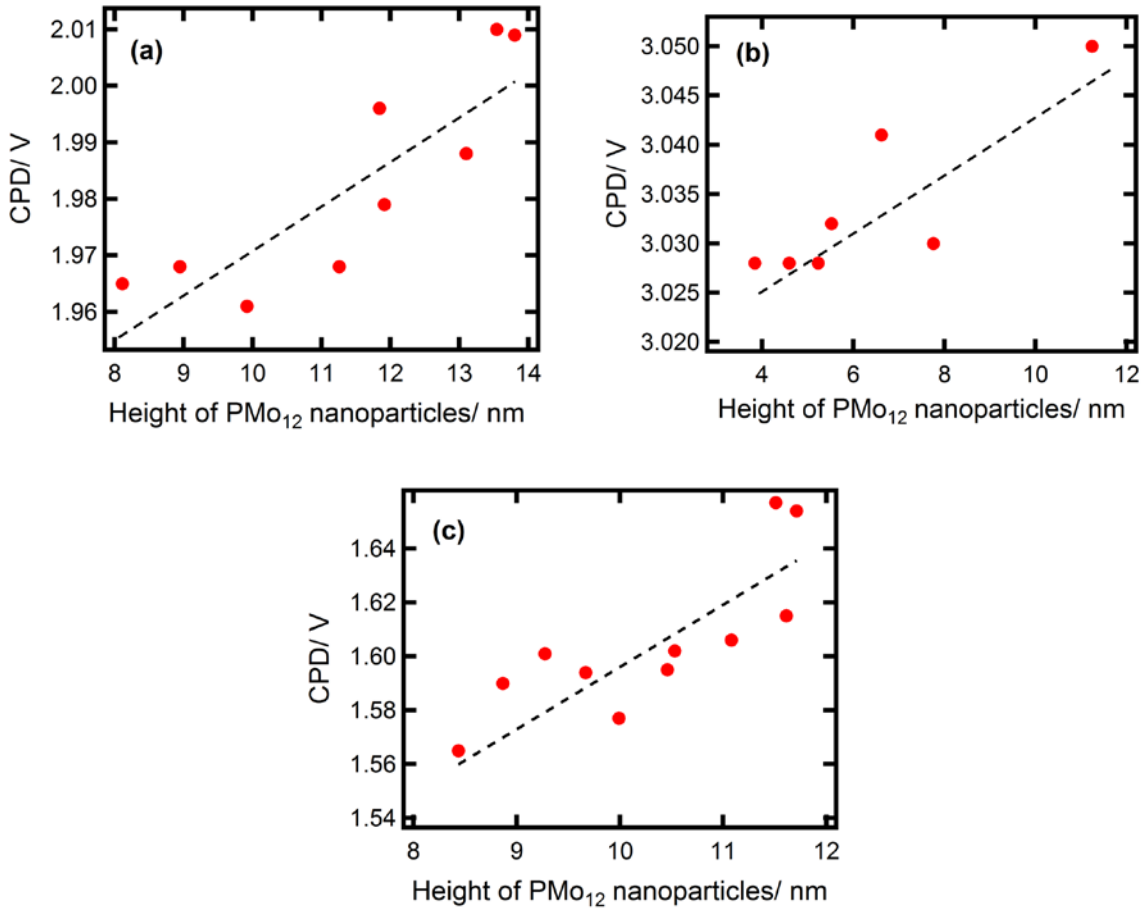

Figure S4. Plots of CPD value against complex height of PMo_{12}/metallic SWNT in three individual complexes. Dashed lines are used just as guides to the eye. In all the three plots, CPD value increases as complex height increases. Therefore, the reproducibility of the relationship between CPD value and height of PMo_{12} particle on metallic SWNT is confirmed.

Table S1. Calculated molecular orbital energies (eV) for PMo_{12} and SWNT

	$H_3PMo_{12}O_{40}$	$H_4PMo_{12}O_{40}^{+}$	$H_4PMo_{12}O_{40}^{\bullet}$	$H_4PMo_{12}O_{40}^{-}$	(13,0) SWNT
LUMO-9	0.0887098	-3.65152	-0.719475	1.80222	-1.50399
LUMO-8	0.0693896	-3.8733	-0.854716	1.63977	-1.68848
LUMO-7	-0.214972	-3.97779	-0.968189	1.58426	-1.68875
LUMO-6	-0.2996	-4.27277	-1.02397	1.53582	-1.69392
LUMO-5	-0.448175	-4.39005	-1.36357	1.21527	-1.75107
LUMO-4	-0.568178	-4.49781	-1.38698	1.2003	-1.86263
LUMO-3	-0.879479	-4.86217	-1.4248	1.05527	-1.86318
LUMO-2	-1.0988	-4.99959	-1.7859	0.882472	-2.28768
LUMO-1	-1.1886	-5.20694	-1.87352	0.737434	-2.76824
LUMO	-1.4531	-5.38436	-2.12523	0.531987	-3.06511
HOMO	-2.17067	-6.25023	-3.14022	-0.398922	-4.26134
HOMO-1	-2.53721	-6.33323	-3.25396	-0.442461	-4.58325
HOMO-2	-2.70511	-6.82467	-3.39165	-0.525728	-5.03115
HOMO-3	-2.97504	-7.03365	-3.70295	-0.984516	-5.63335
HOMO-4	-3.0496	-7.16944	-3.98514	-1.14833	-5.68042
HOMO-5	-3.32281	-7.28645	-4.03657	-1.30915	-5.68124
HOMO-6	-3.4703	-7.48836	-4.10977	-1.39024	-5.70546
HOMO-7	-3.89316	-8.00157	-4.3359	-1.6327	-5.94138
HOMO-8	-4.12256	-8.21246	-4.91659	-2.10645	-5.94192
HOMO-9	-4.18732	-8.32022	-5.11605	-2.29231	-6.03961
HOMO-LUMO gap	0.71757	0.86587	1.01499	0.930909	1.19623
HOMO-LUMO average energy	-1.811885	-5.817295	-2.632725	0.0665325	-3.663225

References for Supporting Information

1 H.Tanaka, T. Yajima, T. Matsumoto, Y. Otsuka and T. Ogawa, *Adv. Mater.*, 2006**, 18**, 1411.

2 T. Yajima, H. Tanaka, T. Matsumoto, Y. Otsuka, Y. Sugawara and T. Ogawa, *Nanotechnology*, 2007**, 18**, 095501.

3 Y. Otsuka, Y. Naitoh, T. Matsumoto and T. Kawai, *Jpn. J. Appl. Phys.*, 2002**, 41**, L742.