Electronic Supplementary Information

One-Dimensional Growth of MoO_x-based Organic-Inorganic Hybrid Nanowires with Tunable Photochromic Properties

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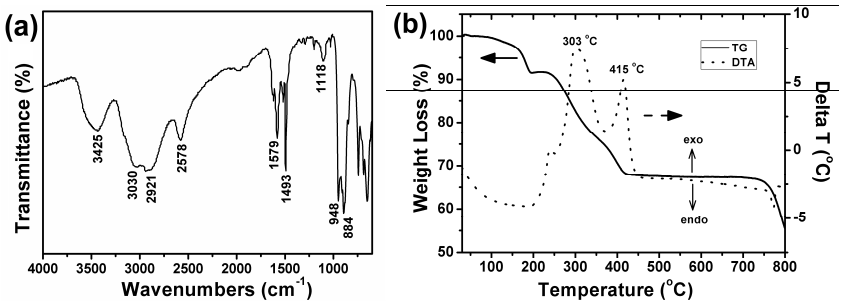

Fig. S1 (a) FT-IR spectrum, (b) TGA and DTA curves of $Mo_3O_{10}(C_6H_8N)_2 \cdot 2H_2O$ nanowires. The absorption bands in IR around 3030 and 2921 cm^{-1} are ascribed ν_{C-H} in benzene ring, and those at 1579 and 1493 cm^{-1} should be assigned to the characteristic vibration of benzene ring. The absorptions at 2578 and 1118 cm^{-1} are due to ν_{NH3+} and ν_{C-N}, respectively. Meanwhile, $\nu_{Mo=O}$ and ν_{Mo-O} in molybdate are clearly detected at 948 and 884 cm^{-1}.

Table S1. Quantum chemical calculation results for MoO_4^{2-} dimerization and combination with $C_6H_8N^+$.

	Entropy (E_f, kcal/mol)
$Mo_2O_7^{2-}$	-416105.3
MoO_4^{2-}	-231617.0
H_2O	-47969.8
H^+	0
$C_6H_8N^+$	-180716.5
$(MoO_4\text{-}C_6H_8N)^-$	-412574.5
dE ($Mo_2O_7^{2-}$)	-841.0
dE [$(MoO_4\text{-}C_6H_8N)^-$]	-241.0

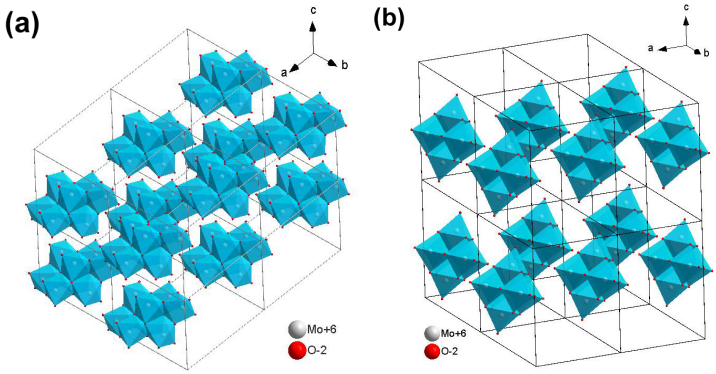

Fig. S2 Polyhedral representation of (a) $Mo_8O_{26}^{4-}$ and (b) $Mo_6O_{19}^{2-}$ clusters in molybdate crystals.

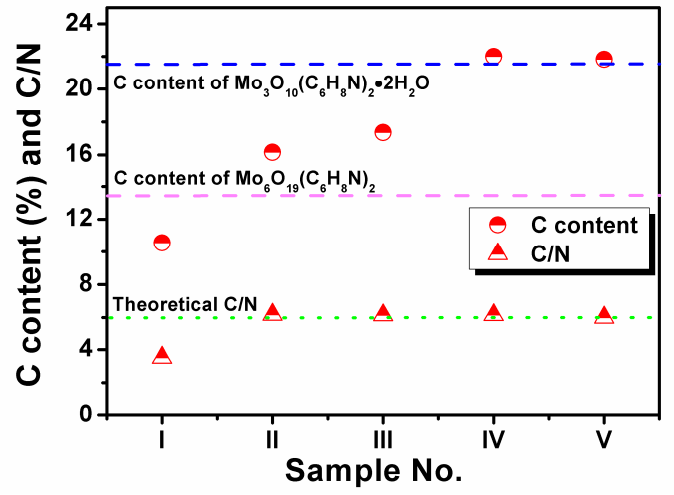

Fig. S3 Carbon content and mole ratio of C/N in the products obtained with feeding aniline/Mo ratios of (I) 0.43, (II) 0.86, (III) 1.72, (IV) 2.58 and (V) 3.00. The carbon content in the product obtained with aniline/Mo ratio of 0.43 is 10.55%, less than the theoretical value of 13.48% in $Mo_6O_{19}(C_6H_8N)_2$. Considering that the C/N molar ratio of 3.52 in such product is also less than that in aniline (C/N=6), some NH_4^+ is believed to be combined with molybdate anion because of inadequate aniline. When aniline/Mo ratio is increased up to 0.86, the C/N molar ratio in all as-obtained products is kept around 6.0, suggesting the combination between NH_4^+ and molybdate anion is totally eliminated by enough anilinium cation. The carbon contents in products generated with aniline/Mo of 0.86 and 1.72 are 16.15 and 17.36%, respectively, which are both slightly higher than the theoretical value in $Mo_6O_{19}(C_6H_8N)_2$, probably due to the presence of some $Mo_3O_{10}(C_6H_8N)_2{\cdot}2H_2O$. When the ratio reaches 2.58 and 3.00, the carbon content is kept ~ 21.5%, consistent with the theoretical value in $Mo_3O_{10}(C_6H_8N)_2{\cdot}2H_2O$.