Electronic Supplementary Information (ESI) for

Transition Metal Selenides as Efficient Counter Electrode Materials for Dye-sensitized Solar Cells

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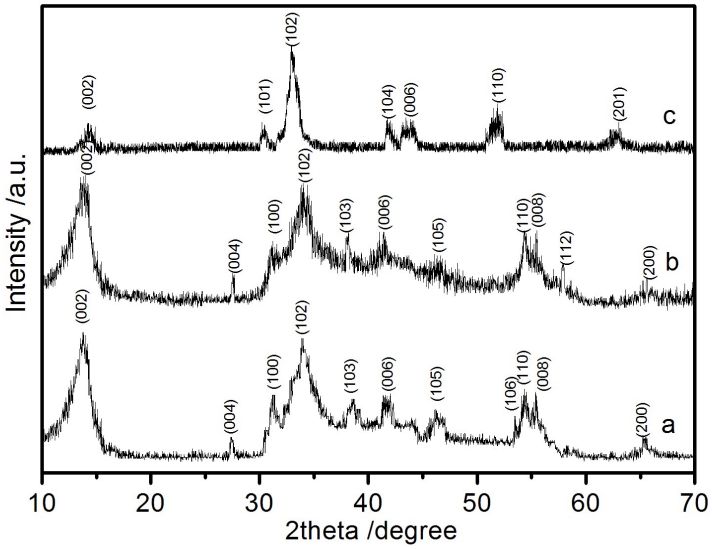

Figure S1 XRD patterns of the synthesized three selenides. (a) $MoSe_2$, (b) WSe_2, and (c) $TaSe_2$.

X-ray diffractograms peak assignments of the synthesized five selenides

In Figure *S*1, for curve a, the diffraction peaks at 13.74°, 27.44°, 31.38°, 34.20°, 37.98°, 42.00°, 47.22°, 53.45°, 55.56°, 56.76°, and 65.30° are assigned to the crystal planes (002), (004), (100), (102), (103), (006), (105), (106), (110), (008), and (200), respectively (29-0914, PDF 2 database) and indicate that the hexagonal $MoSe_2$ was successfully synthesized. For WSe_2, the diffraction peaks at 13.54°, 27.54°, 31.20°, 34.40°, 37.96°, 41.40°, 47.18°, 55.68°, 56.42°, 57.82°, and 65.58° are assigned to the crystal planes (002), (004), (100), (102), (103), (006), (105), (110), (008), (112) and (200), respectively (38-1388, PDF 2 database). For $TaSe_2$, the diffraction peaks at 13.95°, 30.21°, 32.93°, 41.82°, 43.15°, 52.42°, and 62.77° are assigned to the crystal planes (002), (101), (102), (104), (006), (110), and (201) , respectively (19-1303, PDF 2 database).

Table S1 Crystal structures, space groups, lattice parameters, and morphologies of the three TMSs.

Crystal structures	Space groups	Lattice parameters			Morphology
		a(Å)	b(Å)	c(Å)	
$MoSe_2$	P63/mmc(194)	3.287	3.287	12.925	interlaced nanosheets
WSe_2	P63/mmc(194)	3.286	3.286	12.983	nanoplates
$TaSe_2$	P63/mmc(194)	3.436	3.436	12.696	fluffy nanoparticle

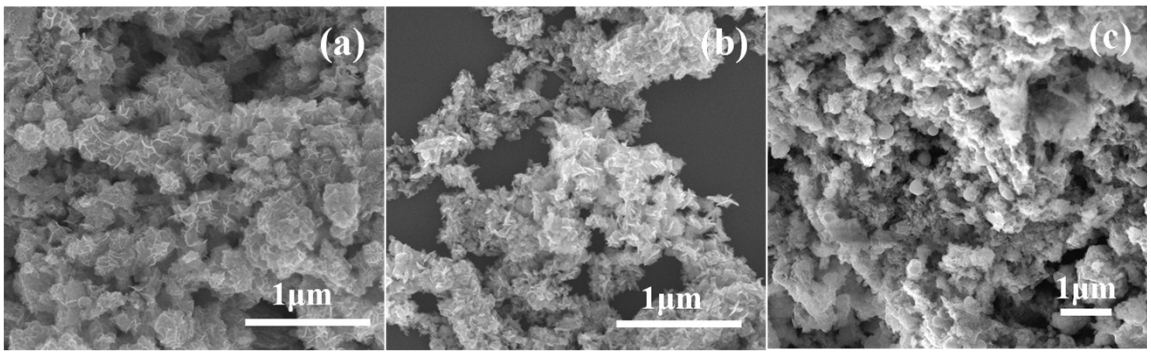

Figure S2 Low-magnification SEM images of the three TMSs: (a) $MoSe_2$, (b) WSe_2, and (c) $TaSe_2$.

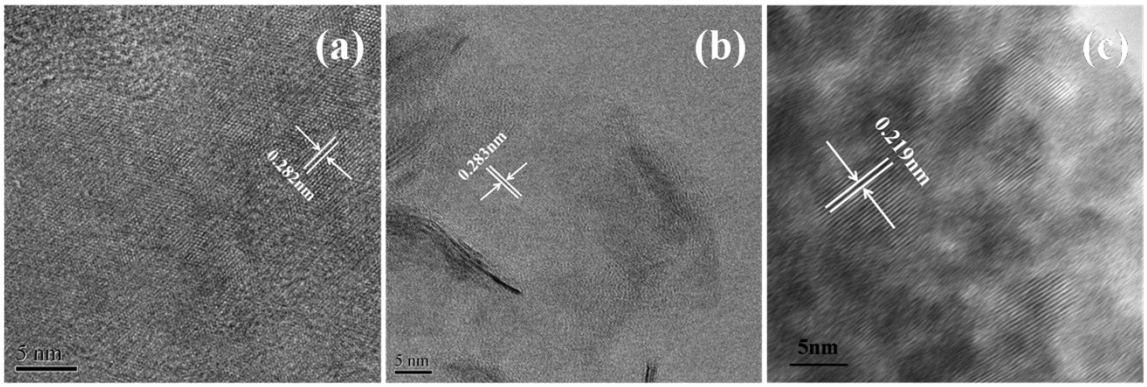

Figure S3 High resolution TEM images of (a) $MoSe_2$, (b) WSe_2, and (c) $TaSe_2$. The high resolution TEM image of $MoSe_2$, WSe_2, and $TaSe_2$ (Figure S3b, c, and d) shows lattice fringes with spacing of 0.282 nm, 0.283nm, and 0.291nm, corresponding to the (100), (100), and (101) planes of hexagonal $MoSe_2$, WSe_2, and $TaSe_2$, respectively.

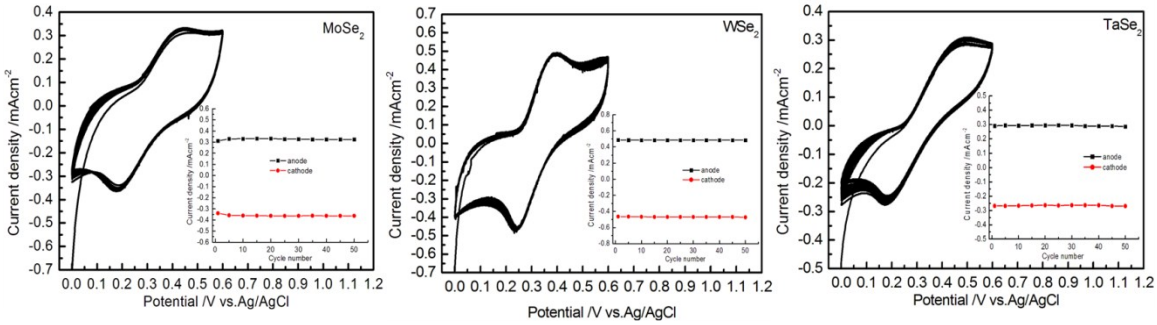

Figure S4 50 consecutive CVs of three TMS-based CE in electrolyte solution containing 2 mM LiI, 0.02 mM I_2, and 20 mM $LiClO_4$; the inset shows the anodic and cathodic peak current densities *versus* cycle time.

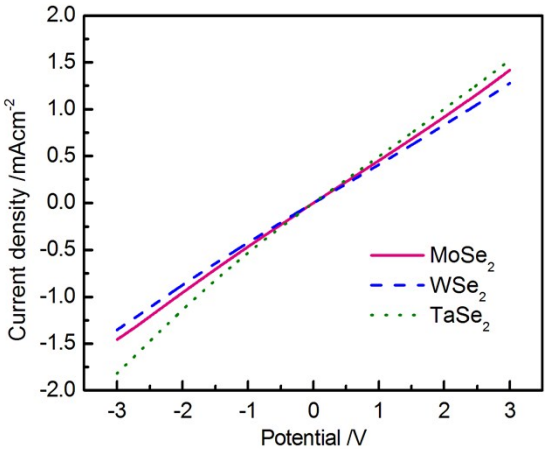

Figure S5 *J-V* curves of CE/CE devices for different TMSs.

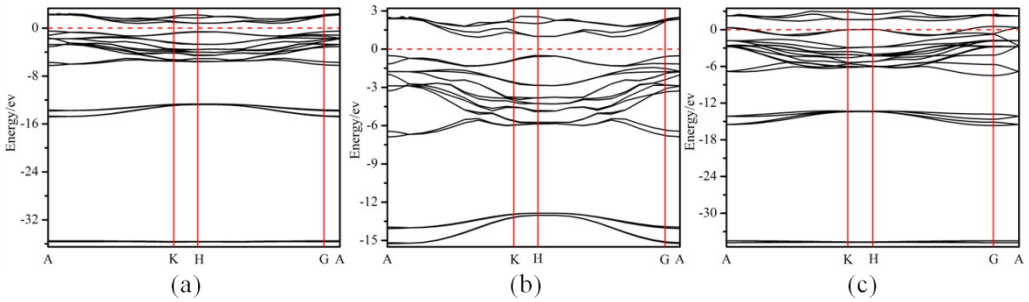

Figure S6 Band structures of the three TMSs: (a) $MoSe_2$, (b) WSe_2, and (c) $TaSe_2$.

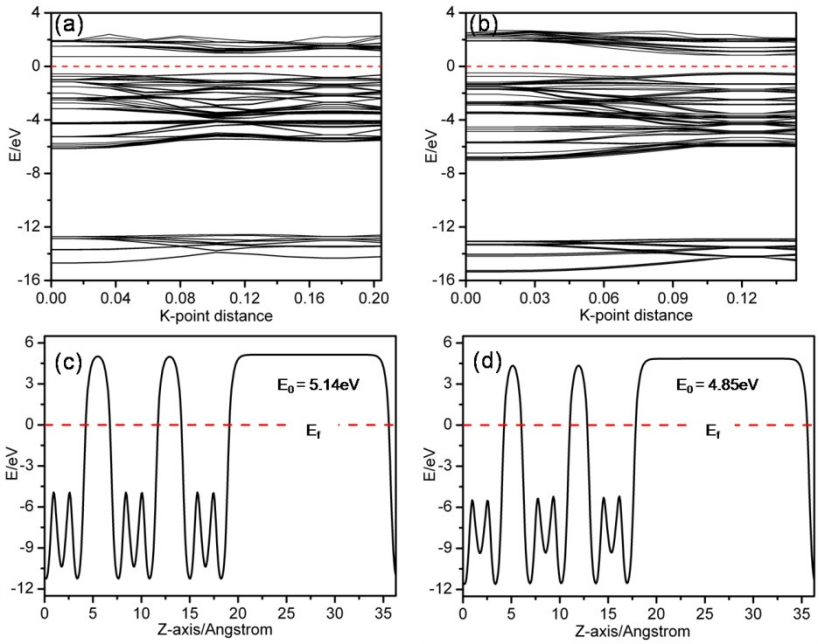

Figure S7 The band structures of (c) $MoSe_2$ and (d) WSe_2 (001) surfaces and electrostatic potential along Z-axis for (a) $MoSe_2$ and (b) WSe_2 (001) surfaces.