Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A. This journal is © The Royal Society of Chemistry 2023

## **Supporting Information**

## Continuous Wet Chemical Synthesis of Mo(C,N,O)<sub>x</sub> as Anode Materials for Li-Ion Batteries

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MoC<sub>0.67</sub>, *Fm*3*m* MoC<sub>0.49</sub>, *P*6<sub>3</sub>/*mmc* 

**Figure S1:** Crystal structures of a) orthorhombic  $Mo_2C$ ,<sup>1,2</sup> b) cubic  $MoC_{0.67}$ ,<sup>3</sup> and c) hexagonal  $MoC_{0.49}$  Mo atoms are depicted in blue, C atoms in black.



Figure S2: General reaction scheme, first step precursor precipitation followed by pyrolysis reaction.

	Carbon	Hydrogen	Nitrogen
	/ mass%	/ mass%	/ mass%
Ideal Mo <sub>2</sub> C	5.89	0	0
Ideal MoOC	9.69	0	0
Ideal Mo₂N	0	0	6.80
PPD/molybdate (9:1) (600°C)	20.85	0.24	0.74
PPD/molybdate (10:1) (600°C)	21.45	0.22	0.59
PPD/molybdate (1:1) (750°C)	0.38	0	2.56
PPD/molybdate (2:1) (750°C)	2.01	0	0.22
PPD/molybdate (5:1) (750°C)	3.19	0	0.14
PPD/molybdate (9:1) (750°C)	22.75	0	0.24
PPD/molybdate (10:1) (750°C)	20.02	0	0.24
PPD/molybdate (15:1) (750°C)	22.62	0	0.30
PPD/molybdate (18:1) (750°C)	23.57	0	0.20
PPD/molybdate (20:1) (750°C)	23.15	0	0.19
PPD/molybdate (25:1) (750°C)	22.86	0	0.23
PPD/molybdate (30:1) (750°C)	22.59	0	0.23

**Table S1:** Elemental analysis of PPD/molybdate precursors after the pyrolysis.



**Figure S3:** Electrochemical performance of pyrolyzed PPD/molybdate hybrid materials. Cyclic voltammograms at different scan rates and potential range between 0.01 V and 3.00 V vs. Li<sup>+</sup>/Li for (a) 1:1 and (b) 10:1 pyrolyzed at 750 °C as well as (c) 9:1 and (d) 10:1 synthesized at 600 °C.



**Figure S4:** Cyclic voltammograms at different scan rates and kinetic fitting to calculate b-values for (a-b) PPD/molybdate (1:1) (750°C); (c-d) PPD/molybdate (10:1) (750°C); (e-f) PPD/molybdate (9:1) (600°C); (g-h) PPD/molybdate (10:1) (600°C).

## Supporting References

- Parthé, E.; Sadogopan, V. The Structure of Dimolybdenum Carbide by Neutron Diffraction Technique. *Acta Crystallogr.* **1963**, *16*, 202–205. https://doi.org/10.1107/s0365110x63000487.
- (2) Norlund Christensen, A. A Neutron Diffraction Investigation on a Crystal of Alpha-Mo<sub>2</sub>C. *Acta Chem. Scand. Ser. A* **1977**, *31*, 509–511.
- (3) 'Rudy, E. .; 'Brukl, C. E. .; 'Windisch, S. . Constitution of Niobium (Columbium)-Molybdenum-Carbon Alloys. *Trans. Metall. Soc. AIME* **1967**, *239*, 1796–1808.