

Quantitative Phase Analysis (QPA) of MXene synthesis product PXRD patterns

Date: 2022-12-06

Tags: Kai Kai 2020 Article 1 Synthesis Optimisation PXRD QPA jEdit TOPAS

Created by: James Bird

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Goal : To use Rietveld refinement with an internal standard to quantify the phases present in MXene synthesis products synthesised in a DoE screening design

Procedure :

- Diffraction patterns of MXene synthesis products mixed with sand (SiO_2) in various proportions were acquired as in [\[Experiment\] XRD analysis of freeze-dried MXene synthesis product with an internal standard - PANalytical X'Pert Pro](#)
- In addition, a LaB_6 calibrant and two phase pure samples of the starting Ti_3AlC_2 MAX phase (Kai Kai 2020 batch, $\approx 98\%$, $< 75 \text{ nm}$) and sand (the internal standard) had diffraction patterns collected under identical conditions (instrument configuration, data collection parameters, sample preparation) with the exception of the lanthanum hexaboride sample which was mixed with ethanol and dropcast on to a zero-background holder.
- Powder diffraction files (PDFs) were found for all standards in the International Centre for Diffraction Data (ICDD) database using X'Pert HighScore Plus in conjunction with PDF-4+
- A structure was defined to represent Ti_3C_2 MXene, based on a model of 10wt% HF direct-etched Ti_3C_2 (<https://pubs.acs.org/doi/abs/10.1021/acs.chemmater.5b04250>)
- All raw scans are treated to ensure intensities are converted to appear as if they'd been collected with a fixed divergence slit (2°) to enable Rietveld refinement
- The instrument, emission and phase pure sample convolutions of line profiles were defined through Rietveld refinement of each of the three standards using jEdit interfacing with TOPAS v5
- Each sample PXRD pattern has its fit optimised within physically justifiable limits to minimize errors

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Results :

Sample Runs 1-3 are not analysed as discussed in [\[Experiment\] XRD analysis of freeze-dried MXene synthesis product with an internal standard - PANalytical X'Pert Pro](#) . All FDS converted data is provided as .xy and TOPAS legible .raw files, with filenameing prefixes Run#_FDS where # = run number. Calibrants and phase pure samples files are named as below.

Sample	As-collected ADS data filename	Converted FDS data filename
Sand (SiO ₂)	JamesBird10mmMaskSpin_SynthOptPXRD__SiO2Sand_20221118.xrdml	Sand_FDS.raw
Ti ₃ AlC ₂	JamesBird10mmMaskSpin_SynthOptPXRD__Ti3AlC2KaiKai2020_20221118.xrdml	MAXPhase_FDS.raw
LaB ₆	JamesBird10mmMaskSpin_SynthOptPXRD__LaB6_20221118.xrdml	LaB6_FDS.raw

First, Rietveld refinement was performed on the LaB₆ standard diffraction pattern to verify that both the instrument function and emission profile can be well defined. All of these refined parameters are then fixed during Rietveld refinement of the phase pure calibrants (Ti₃AlC₂ and SiO₂), to be able to define the structure of each of these phases (including line profile broadening parameters) which are then fixed in subsequent refinements of synthesis product mixtures. All inputs and outputs associated with these refinements are described in the table below: jEdit input and output files are attached along with columnar .txt files detailing each phases corresponding hklm values, d-spacings, 2 θ spacings and scaled intensities (suffixed hklm_d_Th2_IScaled.txt), columnar data of observed intensities, calculated fit intensities and the difference between these (suffixed Yobs_Ycalc_and_Difference.txt), and .png plots of the fitted data. ICDD PDF card numbers are provided for the phase pure samples. R_{wp} and R_{Bragg} values for each refinement/phase are also provided below. Additional outputs include the .par instrument definition, .lam emission profile and .str refined structures of phase pure samples.

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Input	R _{WP}	R _{Bragg}	Output
LaB6_InstrumentFunctionDefinition_FP.inp PDF Card 00-046-1045 Lanthanum hexaboride	9.4488503	2.87406184	LaB6_InstrumentFunctionDefinition_FP.out SynthOpt_PXRD_LaB6.png FPInstrumentFunctionDefinition.par XRD5_Emission.lam LaB6_InstrumentFunctionDefinition_FP_hklm_d_Th2_IScaled.txt LaB6_InstrumentFunctionDefinition_FP_Yobs_Ycalc_and_Difference.txt
MAXPhase_FPFit.inp PDF Card 00-046-1045 Titanium Aluminium Carbide	12.5985114	3.8519441	MAXPhase_FPFit.out MAXPhase_FPFit_hklm_d_Th2_IScaled.txt MAXPhase_FPFit_Yobs_Ycalc_and_Difference.txt MAXPhase.str SynthOpt_PXRD_MAX.png
Sand_FPFit.inp PDF Card 04-012-0632 Hexagonal Beta Quartz	13.6406983	7.13931201	Sand_FPFit.out Sand_FPFit_hklm_d_Th2_IScaled.txt Sand_FPFit_Yobs_Ycalc_and_Difference.txt Sand.str SynthOpt_PXRD_Sand.png

A Ti_3C_2 MXene structure is defined in file 10wt%DirectHFEtched_SmallBoxModel_Wang2016a_Ti3C2.str based on a model of 10wt% HF direct-etched Ti_3C_2 (<https://pubs.acs.org/doi/abs/10.1021/acs.chemmater.5b04250>). All fits of mixtures are carried out using a common .inp jEdit script, named BG_IndividualScan_NoNeg.INP, where various adjustments are made to reduce errors and the known quartz concentration is input as a spike phase. As detailed in the table below, MAX phase, MXene and amorphous concentrations are output, with their associated errors in the adjacent column. The purity of the MXene is calculated (excluding the internal standard) when assuming the amorphous contribution can be attributed to the MXene concentration (MXene purity w/ amorph. / %) and without (w/o). All elemental concentrations are also provided with associated errors in subsequent columns. The final five columns in the table below describe the specific fitting parameters for each Rietveld refinement, where all refinements used a fifth order Cheybshev polynomial to define the fit to the background, minimum and maxium 2θ values are chosen to optimise the fits

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(2theta_min and 2theta_max, respectively) and the order of the spherical harmonics used to improve the fit to account for crystallographic texture in the mixtures is given as '*phase_name* sh'. It can be seen that only in Run 13 were the MAX phase and quartz spherical harmonics were refined again in the mixtures to reduce errors. All other outputs as described above for the phase pure samples (.png, .txt and .out) are also provided, although the run number replaces the phase name in the naming structure.

Run	[MAX] / wt%	err	[MXene] / wt%	err	Amorphous / wt%	err	MXene purity w/ amorph. / %	MXene purity w/o / %	[Ti] / wt%	err	[Al] / wt%	err	[Si] / wt%	err	2theta_min / deg	2theta_max / deg	MAX sh / #	Sand sh / #	MXene sh / #
5	19.47	0.40	11.92	0.76	9.25	0.89	50.65	28.52	25.11	0.46	2.98	0.05	30.57	0.30	6.75	100	Fixed	Fixed	4
6	34.70	0.68	13.03	0.47	37.68	0.99	58.58	15.05	55.85	0.27	7.72	0.07	10.94	0.17	6.75	98.00	Fixed	Fixed	4
8	0.87	0.14	5.32	0.49	14.61	0.51	93.00	24.83	5.15	0.39	0.14	0.02	43.36	0.26	5	100	Fixed	Fixed	2
9	1.31	0.12	6.57	0.41	15.54	0.43	92.32	27.43	6.64	0.33	0.22	0.02	42.38	0.22	5	100	Fixed	Fixed	2
10	1.39	0.11	0.78	0.21	5.33	0.24	78.13	9.97	1.66	0.18	0.20	0.02	45.68	0.11	5	100	Fixed	Fixed	2
11	4.75	0.17	6.07	0.33	8.66	0.37	73.72	30.38	8.66	0.37	0.72	0.02	41.21	0.17	5	98	Fixed	Fixed	4
12	13.77	0.34	5.85	0.5	7.34	0.62	47.45	21.04	15.42	0.37	2.06	0.04	36.85	0.24	5	100	Fixed	Fixed	2
13	2.55	0.66	34.54	4.71	42.50	5.06	90.68	40.65	45.7	2.22	0.61	0.14	16.59	1.46	5	100	6	8	6
14	7.41	0.26	19.14	0.84	3.51	0.90	72.69	61.42	19.68	0.48	1.06	0.04	33.88	0.32	5	90	Fixed	Fixed	4
15	2.95	0.15	3.76	0.35	6.45	0.38	74.74	27.53	5.17	0.27	0.44	0.02	43.39	0.18	5	98	Fixed	Fixed	4
16	22.42	0.91	17.11	1.67	12.45	2.03	54.18	31.36	32.7	2.03	3.55	0.12	25.64	0.60	5	100	Fixed	Fixed	6

Some goodness-of-fit refinement parameters are given in the table below for each of the mixture diffraction patterns where errors were sufficiently minimized: the R-weighted pattern (R_{wp}) of the whole diffraction pattern and R_{Bragg} for each of the three phases.

Run / #	R_{wp}	R_{Bragg}		
		MAX Phase	Sand	MXene
5	24.83	15.82	26.27	4.41
6	17.39	12.76	18.92	4.79
8	25.55	10.89	24.57	4.92
9	21.59	9.38	20.84	3.80

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10	20.17	5.76	16.52	2.85
11	20.65	7.84	16.02	6.60
12	27.16	10.34	30.35	5.31
13	20.26	10.02	25.21	6.57
14	24.68	17.90	22.94	8.51
15	23.33	5.73	19.68	4.14
16	29.64	18.87	19.37	8.34

Notably, despite attempts to fit diffraction patterns of Runs 4 and 7 (which were not excluded from analysis based on sample preparation grounds) the fit errors were too substantial to be considered useful.

Attached files

Run12_FDS.raw

sha256: a5622a0452f44f8fe6aef49920eeb76d7a7caa61e2acbbef12d95b0fb4ef0907

Run11_FDS.raw

sha256: 5abf692ba0669bc727abd415f806b434eb9a9dc71776c2b3eb964bb860fc6672

Run13_FDS.raw

sha256: b3cb491f7a5bad7c995abf4a072cbe1a1fcc09c6fccb16f4b97327e60545ea15

Run14_FDS.raw

sha256: 2aa1b378d0649b044d5ebcb71e95c6b8183fb74ccaa317fa7d7bda949eef3663

Run15_FDS.raw

sha256: b868faefcdb1810029825094f19deade0290a32075777dba58b3f91304f826c4

Run16_FDS.raw

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sha256: 696ee7e6c9f5f5be345cdd196cd14b76b1a2125bb251b68a4acf9a642e58355b9

Sand_FDS.raw

sha256: d3e79c50efa54a5bec01c82b855bbefc97868f78898e7807d470097b7aa704cf

LaB6_FDS.raw

sha256: 57509d57852066bee050e455e811f197a910838edd3b0baa130f1c58eb47d6e7

MAXPhase_FDS.raw

sha256: 93e45df47256211374c4c21a0d6d2495e0a5dd6e5f76ddb9795b7222e3145182

Run4_FDS.raw

sha256: c6371beac28cc1fb5892ff072a3b7b00b45e749fc33ef9322a1369997ecd58c0

Run5_FDS.raw

sha256: cdd8e5f0457063d0c5618e0b3d0dd47f25cdc5caf055a5aa919dd8e05ed07081

Run6_FDS.raw

sha256: 349b3305789ba91904b5043b36b055fa557ad7a2c735b1417fd25395ca4cf2c1

Run7_FDS.raw

sha256: b9f2b418d36d3ece8dc5c12b8e4cb95e83ea33e2d5f72df0d786e4bf1a7265d6

Run8_FDS.raw

sha256: 74a8d463a0ee6129e0e55b71f52ce4b584fb86be248f4236f589734c38739784

Run9_FDS.raw

sha256: 7b9b2520a15d96ac02a3840c48377f0b45654bdd74368b9ba258c10527622694

Run10_FDS.raw

sha256: 228ac0836326e7e66dcc5e854b2c02e4c3aefbd76e30a4e3c6ff77c47871bb1a

JamesBird10mmMaskSpin_SynthOptPXRD__SiO2Sand_20221118.xrdml

sha256: c313cc78baf60fbd10b41b8dc3674e1be1cfaebf60c96d91d770553454ae7fcf

JamesBird10mmMaskSpin_SynthOptPXRD__Ti3AlC2KaiKai2020_20221118.xrdml

sha256: cd6b2810e9aa33a51f00517e8346f0348529b7bfc42d44da0403cda88c34e489

JamesBird10mmMaskSpin_SynthOptPXRD__LaB6_20221118.xrdml

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sha256: 0ece436eb7eca180ae34c678408feee14c7f0f2d43e053012d95d977fa7e6ab5

Run11_FDS.xy

sha256: 1a51e6b554140df4ba90a0193dbca2aea75d5a516593147d89aba3e164b34ff4

Run12_FDS.xy

sha256: c23d6687501c47c57c0096b3ecd1d6c1d6d6ae3215982d39d2ce13cf93c18517

Run13_FDS.xy

sha256: 7d99e7e71acbcf0106fefa7b2331eef651b2fb22b9f8583290d9367ac6e5689d

Run14_FDS.xy

sha256: e2cec2fe390a58506f683523b7b320da020b743c4b115e09aeff6e846c592236

Run15_FDS.xy

sha256: 05f81bc120d31d680660c59c21cbe152759a1df4aa9888a2d9e969d597cf16dd

Run16_FDS.xy

sha256: a4916db12c319c9dfd92e9540b083dc4a68b8b01d7761372c00d57ab60e9a0bb

Sand_FDS.xy

sha256: 2fa9ed504c2890d40c441e0accc0f095e03657d48827dd1bc214ce9a393c9e80

LaB6_FDS.xy

sha256: 3e437ab85df37f70dfc0665e6f3cee37b9ad9d437c054666f1a4b633be7ec9ae

MAXPhase_FDS.xy

sha256: 246e31b70c424cc6c2dedc1187f1866b335c15095fc7c0d402cc86aec8f7e10d

Run4_FDS.xy

sha256: 77d4f8184ae12a9b961584afb6091f9698f475c4a12f55e4b73f31cb65326fef

Run5_FDS.xy

sha256: 32219c61c61402730f7804eeac01c73bf78ee66cea1380d75edc096efb318ac4

Run6_FDS.xy

sha256: 16e295df7fe8808e1bc12e94a239f4a0a5eee48c396e31513b0b8204944f9ff9

Run7_FDS.xy

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sha256: 4f88dc534b5b739f456ebe475ff1e16ef3c77fe99408abffad88f5b92fd4ea83

Run8_FDS.xy

sha256: cf413e42180dc6910b83ca6e5047b30054516d9e095b374c2d3c39eb2415e015

Run9_FDS.xy

sha256: 4d462f21ce4bc8eade0c73b40648b283454577586293dc184b259a3327ed3836

Run10_FDS.xy

sha256: 66e23ff2860cf4edbe0c739139a6196999014584bee59e7b1c6e434930538479

LaB6_InstrumentFunctionDefinition_FP.inp

sha256: d8db029d04e89ea734ef23e04243510f0fd1a17bef04629ddac87ef0f1154492

LaB6_InstrumentFunctionDefinition_FP.out

sha256: 9b4b8f2b5e7354a45f9f0c8f1fe2344339a53a24d1286ecd2da9da772e42ebf8

FPInstrumentFunctionDefinition.par

sha256: b5b9afc0a6bd6e2693608ea599443182f0ca82dc821a0c158194887fa4fb9494

MAXPhase_FPFit.inp

sha256: 2366bfab8ee26467406ef3ddaa62b69af3477e0c9386d16845ec1827f4f8c4fe

MAXPhase_FPFit.out

sha256: 1e054ddc26f6aede500d9b14a2af89f05b9b003604a472a08e132f72cc509023

LaB6_InstrumentFunctionDefinition_FP_hklm_d_Th2_IScaled.txt

sha256: 5fb3f6221537d0e7c737d9c22429944de7e6aad02172024fef9fff9835532f09

LaB6_InstrumentFunctionDefinition_FP_Yobs_Ycalc_and_Difference.txt

sha256: 0f547eb66c5037829d8adde194ab18de2b76922a8149c6bcd1a2b8e4a257ee96

XRD5_Emission.lam

sha256: 4d37b1ad016329dc6f1f57d6847d6d1459219f7af1013646b3380d3eacae8d4d

MAXPhase_FPFit_hklm_d_Th2_IScaled.txt

sha256: d97f669d999aff13741e0476e21f9b321e833d70abcc6ea82a6a7a169e4633c6

MAXPhase_FPFit_Yobs_Ycalc_and_Difference.txt

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sha256: e3b5d0bb412ea505513bff420771a88d63c6cabb5ce28486d5b2b73cf0465a12

MAXPhase.str

sha256: d3c9b9fa50bb8e41f510e93738f90eb3cf7b463db257a9fe3e282d985fc46d6e

Sand.str

sha256: e996ae09cf385430062b1d9d4e97516683677c1692f25277a27267263892ada8

Sand_FPFit_hklm_d_Th2_IScaled.txt

sha256: ddc33b9e76c20c26268ae57fcd7dc9f870732e70f22c969aca39cd5aaab7973

Sand_FPFit_Yobs_Ycalc_and_Difference.txt

sha256: c173cee944a333a9e9ff0db0a2506c4238ea6d6128c2ef79a0273a77de8290e7

Sand_FPFit.inp

sha256: f3ee4c37580021efa592ad739fe290a4ef8204885b039423fec08609cc78008b

Sand_FPFit.out

sha256: 6c9d51928ab64979f76a3a80145b7415c2542c507a3bc2a8344ebe4f93a75927

10wtDirectHFEtched_SmallBoxModel_Wang2016a_Ti3C2.str

sha256: f4b9f5449f5ac0c6e48ab29ce1c9978407ca3cf5bfbb921b0d6588af96d685ac

Run8_hklm_d_Th2_IScaled.txt

sha256: d791579ad151e57e5fc54275551dd05127728cd3970a355e01e328c4ccfbcb7

Run6_Yobs_Ycalc_and_Difference.txt

sha256: 28d3326b197e8bb60b890e326b38baa20deab841d9a670258a67787d6d45b0e8

Run8_Yobs_Ycalc_and_Difference.txt

sha256: 1a3a45bf25948a5c5d0d8354a4d3119cfc91f80db395c5b945a5f19f92e868b6

Run9_hklm_d_Th2_IScaled.txt

sha256: 65f0c451659f741250749cbc0175b8e1815e30ada7add7d125cf85400824fac2

Run10_hklm_d_Th2_IScaled.txt

sha256: 659c283d9e3e0641a5273feb658a8ad56a7d989f98e8d51452a6906a37b775c1

Run9_Yobs_Ycalc_and_Difference.txt

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sha256: 456ae5af6a04c97628b9a9d3e326417c9cea5eb89c8389249387fd1b1f1376a0

Run10_Yobs_Ycalc_and_Difference.txt

sha256: 41bc95c123ac1f19d1d4e7261ef8b18f09fe0b9f9675fdd894ab5eebd1ce469e

Run11_hklm_d_Th2_IScaled.txt

sha256: 95bc64f218971162c746e7e7393cb8a7cd5dfe03b2e93397ceb58acad2ef11dd

Run12_hklm_d_Th2_IScaled.txt

sha256: 2063dfa457588818f3210baf05783ed71de4b079c46877d95cb0e9ce8412f522

Run11_Yobs_Ycalc_and_Difference.txt

sha256: 0d7af95f62a15e392725671b82fe71a81959c72ce19299650ebc11e557070c94

Run13_hklm_d_Th2_IScaled.txt

sha256: 90a81643ab44449af58e0223c62d4815000d944a5c28f4c6a96f8f0f0af9cbe7

Run12_Yobs_Ycalc_and_Difference.txt

sha256: fd9e5f93426fba5bb9ece5dbe9a670c1c0e53ad720a1774eb3747f4a52fb2a50

Run13_Yobs_Ycalc_and_Difference.txt

sha256: c1d6ec330ed0e8625fb0862f514ba7dad20f00fc64af97bc697763431000f387

Run14_hklm_d_Th2_IScaled.txt

sha256: 95724a9737b5ff4856d32e217de70e16eb943aa83ec4fd07d250a6a2c775243d

Run14_Yobs_Ycalc_and_Difference.txt

sha256: 3a2ae7fc7b6a038dd69b3dae472cfe28ca042f21795c0ccecd79085c8ccf5309

Run15_hklm_d_Th2_IScaled.txt

sha256: 15f56c5ad345d95580a04ed70e3611ed8e30709875765eb12a5c0a9801e3f7d1

Run15_Yobs_Ycalc_and_Difference.txt

sha256: 45ada0581c0f0be0e6970a4bc2195a84def18ee84dc0507c0127b97589131936

Run16_hklm_d_Th2_IScaled.txt

sha256: 8b413120a70a3127708ef7a2cc319b44cd5d310b67e26418cf8081e6a03ee03c

Run5_hklm_d_Th2_IScaled.txt

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sha256: 9806b60688a9b2f8a05e09489869ed9ab4f4c7cd3936cb6c3791ee34545c518f

Run16_Yobs_Ycalc_and_Difference.txt

sha256: 1be00a6aea013f29f64d1929fb3610cd0e975623a3e4495a77bb7c65742fd6a5

Run6_hklm_d_Th2_IScaled.txt

sha256: 4bb570182bc07c8396c6ac2155da38a3731acffb034b7531e619a197848f4cd7

Run5_Yobs_Ycalc_and_Difference.txt

sha256: 8a89322bf2359706ba137a6ef2525cd9d7875f6640228da206c75690d3155be4

Run9.out

sha256: 6a02d19583134248d61afb50b07315415ddc7bc1e311d4bb7c0190965947d723

Run10.out

sha256: 0c628d12ec60aa6ffdf871270b9c7e98dde26affaf7ca4e931a4320ce57d0b4c

Run11.out

sha256: e51dc9ee65543b8023c30250df16fd5e40824e9153921a96a85fd5bba827f1bf

Run13.out

sha256: 62063b0d2a1fc92391c929dbea9f61c5cdd52ef59e474267261431778b319f0a

Run12.out

sha256: c90bf620a9daf1f851db016b4547b9cd51631ab2ec0c729b3e9e7eec2ec07fc0

Run14.out

sha256: adfeaf94760c6132db69921171dcae468a5ce27b03bd4864371f7503a109f082

Run15.out

sha256: 71c3fc31af44b1049658356801d1d9f01d223a8d28ef8d65b053fcaa6d512a93

Run16.out

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Run5.out

sha256: 6f4147747de558b9f0ba2ba9f5b0d599ccea53b2ba4491e92877aba671cacba3

Run6.out

Quantitative Phase Analysis (QPA) of MXene synthesis product PXRD patterns

Date: 2022-12-06

Tags: Kai Kai 2020 Article 1 Synthesis Optimisation PXRD QPA jEdit TOPAS

Created by: James Bird

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sha256: 13757d3dae40417ef7c8f29f12f273ef1fb366145395d215fbc8d28f611f5b8d

Run8.out

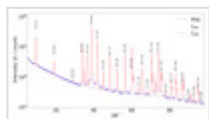
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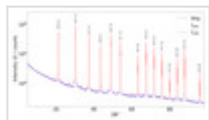
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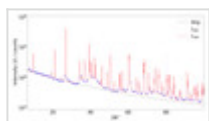
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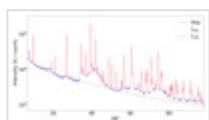
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SynthOpt_PXRD_Run6.png

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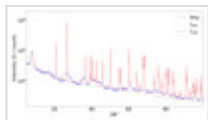
Quantitative Phase Analysis (QPA) of MXene synthesis product PXRD patterns

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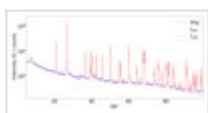
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SynthOpt_PXRD_Run10.png

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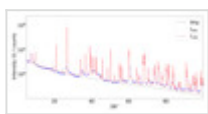
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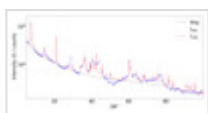
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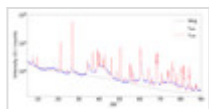
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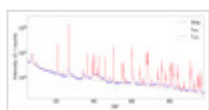
Created by: James Bird

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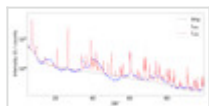
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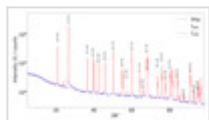
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SynthOpt_PXRD_Sand.png

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