crystals

MDPI

Supplementary Materials

Crystallization of ApoA1 and ApoE4 Nanolipoprotein Particles and Initial XFEL-Based Structural Studies

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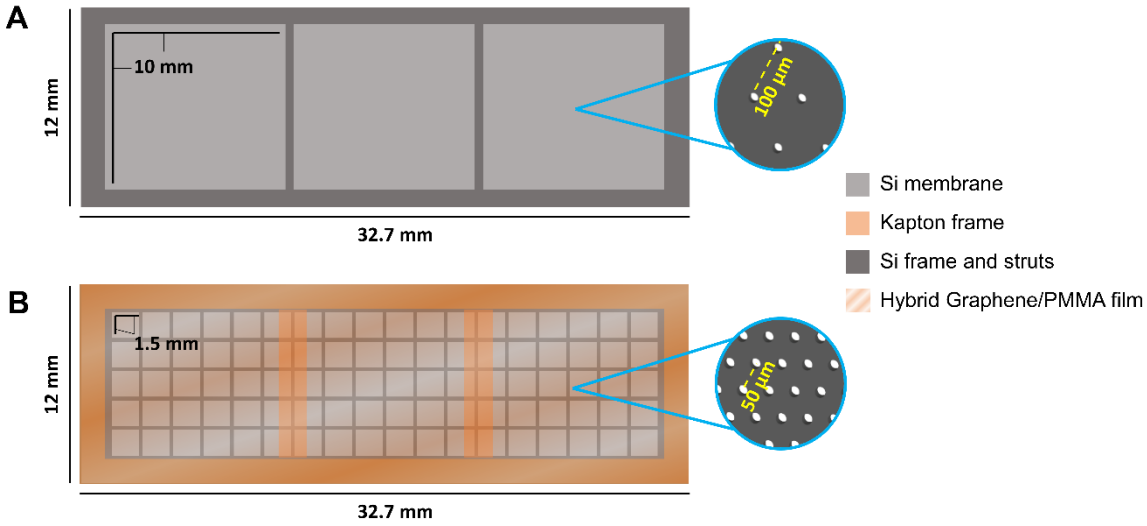

Figure S1. General design of two styles of chips used in experiments at MFX in near 100% relative humidity (**A**) and the Graphene/PMMA enclosed chips used at CXI in vacuum (**B**). Chips in (**A**) utilized a 3 × 1 large-window layout with 100 µm hexagonal pore spacing and samples were measured with no enclosing layers. Chips in (**B**) utilized an 18 × 5 small-window layout with 50 µm hexagonal pore spacing and were enclosed with Graphene/PMMA films supported by the chip and a Kapton frame.

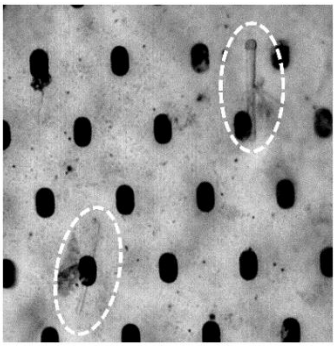

Figure S2. Optical microscopy image showing NLP crystals deposited on a single Graphene/PMMA film supported by the hexagonal pore patterned Si membrane of the chip and enclosed in a second Graphene/PMMA film. After enclosure, the assembly was exposed to vacuum for 30 min without any apparent desiccation of the enclosed sample. Rod-shaped crystals are circled in white.

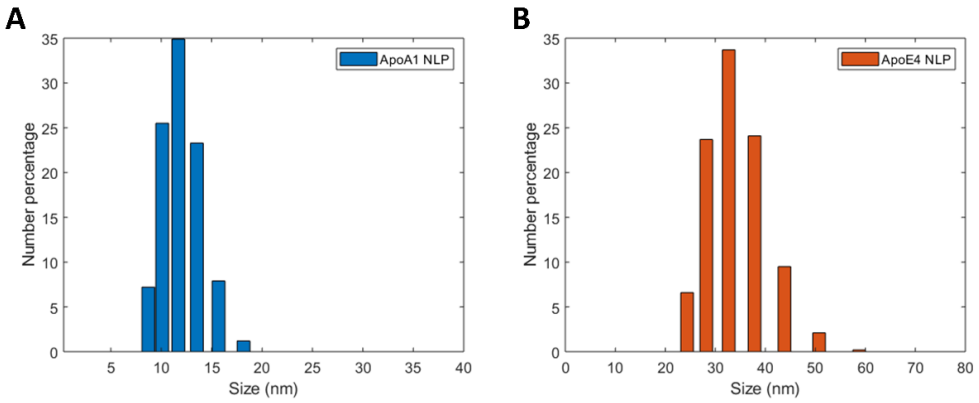

Figure S3. Size distributions of ApoA1 (**A**) and ApoE4 (**B**) NLP hydrodynamic radii as measured by dynamic light scattering (DLS).

Table S1. Salt composition for all hits from the HWI soluble and membrane screens for ApoA1 and ApoE4.

		ApoA1 NLPs				ApoE4 NLPs			
CATION	**charge**	**Total hits (out of 165)**	**% of total hits**	**total cocktails containing this component**	**% of hits in total cocktails containing this component**	**Total hits (out of 237)**	**% of hits**	**total cocktails containing this component**	**% of hits in total cocktails containing this component**
Magnesium	+2	57	34.55	330	17.27	123	51.90	394	31.21
Sodium	+1	49	29.70	1186	4.13	58	24.47	1191	4.86
Ammonium	+1	29	17.58	750	3.87	43	18.14	750	5.73
Lithium	+1	13	7.88	243	5.35	21	8.86	243	8.64
Potassium	+1	10	6.06	365	2.74	13	5.49	365	3.56
Calcium	+2	6	3.64	117	5.13	N/A	N/A	N/A	N/A
Barium	+2	1	0.61	1	100.00	N/A	N/A	N/A	N/A
Rubidium	+1	1	0.61	25	4.00	N/A	N/A	N/A	N/A
ANION	charge	Total hits (out of 165)	% of total hits	total cocktails	% hits/total cocktails	Total hits (out of 237)	% of hits	total cocktails	% hits/total cocktails
Chloride	−1	89	53.94	1011	8.80	136	57.38	1074	12.66
Sulfate	−2	26	15.76	570	4.56	42	17.72	570	7.36
Citrate	−3	24	14.55	541	4.44	41	17.30	541	7.57
Phosphate	−3	15	9.09	408	3.68	22	9.28	408	5.39
Bromide	−1	5	3.03	101	4.95	1	0.42	101	0.99
Acetate	−1	4	2.42	316	1.27	5	2.11	318	1.57
Nitrate	−1	4	2.42	111	3.60	3	1.27	111	2.70
Carbonate	−2	3	1.82	26	11.54	N/A	N/A	N/A	N/A
Molybdate	−2	2	1.21	20	10.00	2	0.84	20	10
Thiocyanate	−1	N/A	N/A	N/A	N/A	1	0.42	50	2
Thiosulfate	−2	N/A	N/A	N/A	N/A	1	0.42	14	7.14

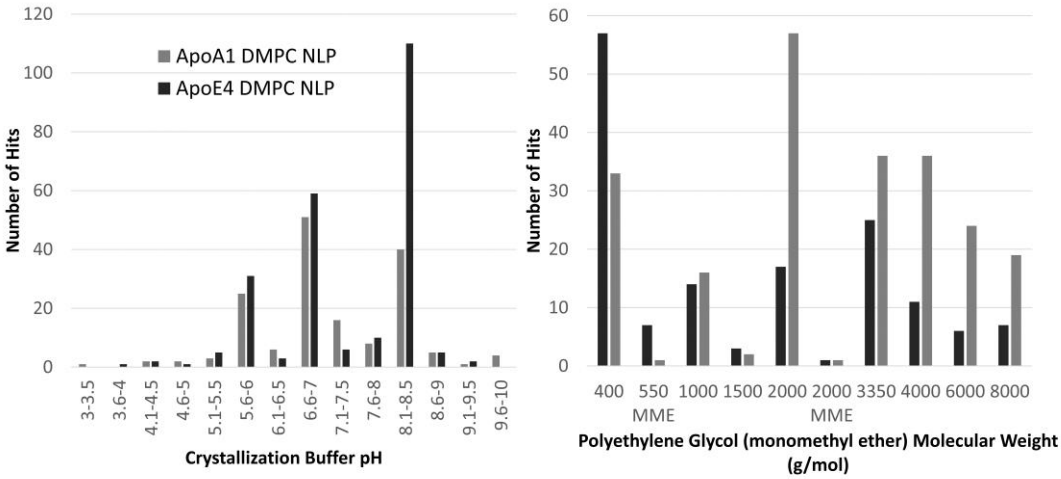

Figure S4. Crystallization buffer conditions and polymer precipitant composition for all hits from the HWI soluble and membrane screens for ApoA1 and ApoE4.