

**Table S4.** Coefficients of the regression models and analysis of variance obtained for each key property in the H-aggregates.

	$BI$ (cubic)	$\rho_{rd}$ (special cubic)	$\sqrt{WA_{24}}$ (special cubic)	$\sqrt{S}$ (quadratic)
K	-5.5	1.9	3.4	4.2
H	-549.7	2.9	7.3	6.1
C	-485251.5	-232.0	-3.0	420.4
N	-12382.6	-400.5	1431.2	-824.8
cubic (K,H)	-714.3	-	-	-
cubic (K,C)	-262661.4	-	-	-
cubic (K,N)	-13944.3	-	-	-
cubic (H,C)	-291698.1	-	-	-
cubic (H,N)	1241.9	-	-	-
cubic (C,N)	376049.2	-	-	-
K:H	1028.6	3.1	-18.2	-3.2
K:C	747087.1	242.0	13.6	-473.0
K:N	25609.1	422.4	-1497.9	844.8
H:C	773019.2	283.4	-148.7	-574.2
H:N	13952.7	450.8	-1644.1	905.1
C:N	660327.3	5287.4	-6628.9	538.4
K:H:C	-546064.2	-297.6	574.7	-
K:H:N	-15435.9	-61.1	335.0	-
K:C:N	-429441.4	5171.9	5981.4	-
H:C:N	-460743.9	-4876.0	4373.7	-
F-statistic	14.48	182.4	107.5	111.5
p-value	8.942e-07	< 2.2e-16	< 2.2e-16	< 2.2e-16
R <sup>2</sup>	0.8822	0.986	0.976	0.9684