Supporting Information for

Backbone flexibility of extended metal atom chains. Ab initio molecular dynamics for $Cr_3(dpa)_4X_2$ ($X = NCS^-$, CN^-, NO_3^-) in gas and crystalline phase.

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Table S1. Relevant mean distances (*d*, in Å) and angles (*a*, in degrees) from the molecular dynamics of $Cr_3(dpa)_4(CN)_2$. Average values are reported for the group of symmetric (Δdist < 0.15 Å) and asymmetric (Δdist > 0.15 Å) structures. X-ray values are shown. Previous DFT optimized structural parameters are shown for comparison.

	Gas phase MD		Crystal MD		X-ray[1]	Static DFT Opt[2]
	Symmetric	Asymmetric	Symmetric	Asymmetric		
$d(Cr_1\text{-}Cr_2)$	2.314	2.275	2.358	1.928	2.370	2.370
$d(Cr_2\cdots Cr_3)$	2.332	2.531	2.379	2.695	2.370	2.370
$d(X\text{-}Cr_1)$	2.187	2.198	2.323	2.452	2.284	2.186
$d(X\text{-}Cr_3)$	2.176	2.135	2.201	2.299	2.284	2.186
$a(N\text{-}C\text{-}Cr_1)$	164.6	165.5	145.3	145.6	173.7	180.0
$a(N\text{-}C\text{-}Cr_3)$	164.2	164.8	139.7	147.6	173.7	180.0

(1) John F. Berry; F. Albert Cotton; Tongbu Lu; Carlos A. Murillo; Brian K. Roberts; Wang, X. Molecular and Electronic Structures by Design: Tuning Symmetrical and Unsymmetrical Linear Trichromium Chains. *J. Am. Chem. Soc.* **2004**, *126* (22), 7082–7096.

(2) Spivak, M.; Arcisauskaite, V.; Lopez, X.; McGrady, J. E.; de Graaf, C. A Multiconfigurational Approach to the Electronic Structure of Trichromium Extended Metal Atom Chains. *Dalt. Trans.* **2017**, *46* (19), 6202–6211.