Supplemental Information

Examples of textual perturbations of MSE-MCQs questions and crystal structure descriptions from LLM-Prop band gap dataset

Degradation Type	MSE-MCOs Example Prompt	LLM-Pron Example Prompt
Original	32 g of solid sugar is added to 68 g of liquid water at room temperature	Be, AlMn crystallizes in the cubic $\overline{E}43m$ space group. Be is bonded to
Original	and allowed to reach equilibrium. No solid sugar is observed within	six equivalent Be three equivalent Mn and three equivalent Al atoms
	the container. The temperature is then lowered to a temperature T1 and	to form a mixture of edge face and corner-sharing BeMn ₂ BecAl ₂
	allowed to reach equilibrium. At temperature T1 it is observed that only	cuboctahedra There are three shorter (2.12 Å) and three longer (2.17 Å)
	solid sugar and solid water (ice) exist. There is no solubility of sugar	Be–Be bond lengths. All Be–Mn bond lengths are 2.51 Å. All Be–Al
	in solid water, nor of water in solid sugar. How many grams of ice are	bond lengths are 2.52 Å. Mn is bonded in a 16-coordinate geometry to
	present in this container?	twelve equivalent Be and four equivalent Al atoms. All Mn-Al bond
	(a) 68 g	lengths are 2.63 Å. Al is bonded in a 16-coordinate geometry to twelve
	(b) 32 g	equivalent Be and four equivalent Mn atoms.
	(c) 36 g	
	(d) None of these options	
Unit Mixing	0.032 kg of solid sugar is added to 0.068 kg of liquid water at room tem-	N/A
	perature and allowed to reach equilibrium. No solid sugar is observed	
	within the container. The temperature is then lowered to a temperature	
	that and allowed to reach equilibrium. At temperature 11, it is observed that any solid sugar and solid sustant (iso) avist. There is no solubility	
	of sugar in solid water, nor of water in solid sugar. How many grams of	
	ice are present in this container?	
	(a) 0.150 lbs	
	(b) 32000 mg	
	(c) 36000 mg	
	(d) None of these options	
Sentence Reordering	At temperature T1, it is observed that only solid sugar and solid	Be ₄ AlMn crystallizes in the cubic $\overline{F}43m$ space group. All Be–Al bond
	water (ice) exist. No solid sugar is observed within the container. The	lengths are 2.52 Å. All Be–Mn bond lengths are 2.51 Å. All Mn–Al
	temperature is then lowered to a temperature T1 and allowed to reach	bond lengths are 2.63 Å. Mn is bonded in a 16-coordinate geometry
	equilibrium. There is no solubility of sugar in solid water, nor of	to twelve equivalent Be and four equivalent Al atoms. There are
	water in solid sugar. 32 g of solid sugar is added to 68 g of liquid	three shorter (2.12 Å) and three longer (2.17 Å) Be–Be bond lengths.
	water at room temperature and allowed to reach equilibrium. How	Al is bonded in a 16-coordinate geometry to twelve equivalent Be
	many grams of ice are present in this container?	and four equivalent Mn atoms. Be is bonded to six equivalent Be,
	(a) 68 g	three equivalent Mn, and three equivalent Al atoms to form a mix-
	(b) 32 g	ture of edge, face, and corner-sharing BeMn ₃ Be ₆ Al ₃ cuboctahedra.
	(c) 36 g	
Cymonym Donlogomont	(d) None of these options	N/A
Synonym Replacement	52 g of solid sucrose is added to 68 g of H_2O at allocated conditions	N/A
	the container. The temperature is then reduced to a temperature T1 and	
	allowed to reach equilibrium. At temperature T1 it is observed that only	
	solid sucrose and crystalline water (ice) exist. There is no dissolution	
	of sucrose in crystalline water, nor of water in solid sucrose. How	
	many grams of ice are present in this container?	
	(a) 68 g	
	(b) 32 g	
	(c) 36 g	
	(d) None of these options	
Distractive Information	One morning, the mothers and fathers were ready as usual in the	One morning, the mothers and fathers were ready as usual in the
	main square of Four Houses waiting for the red bus. But this was no	main square of Four Houses waiting for the red bus. But this was no
	ordinary day, for the red bus was twenty minutes late. Very slowly,	ordinary day, for the red bus was twenty minutes late. Very slowly,
	from exhaustion. There was no way he could take the children to	from exhaustion. There was no way he could take the children
	school today. Then the teacher asked:	to school today. Then the teacher asked: Ber AlMn crystallizes in
	32 g of solid sugar is added to 68 g of liquid water at room temperature	the cubic $\overline{F}43m$ space group. Be is bonded to six equivalent Be, three
	and allowed to reach equilibrium. No solid sugar is observed within	equivalent Mn, and three equivalent Al atoms to form a mixture of edge.
	the container. The temperature is then lowered to a temperature T1 and	face, and corner-sharing $BeMn_3Be_6Al_3$ cuboctahedra. There are three
	allowed to reach equilibrium. At temperature T1, it is observed that only	shorter (2.12 Å) and three longer (2.17 Å) Be–Be bond lengths. All
	solid sugar and solid water (ice) exist. There is no solubility of sugar	Be–Mn bond lengths are 2.51 Å. All Be–Al bond lengths are 2.52 Å.
	in solid water, nor of water in solid sugar. How many grams of ice are	Mn is bonded in a 16-coordinate geometry to twelve equivalent Be and
	present in this container?	four equivalent Al atoms. All Mn–Al bond lengths are 2.63 Å. Al is
	(a) 68 g	bonded in a 16-coordinate geometry to twelve equivalent Be and four
	(b) 32 g	equivalent Mn atoms.
	(c) 36 g	
	(d) None of these options	
Superfluous Information	32 g of solid sugar is added to 68 g of liquid water at room temperature	Be ₄ AlMin crystallizes in the cubic $F43m$ space group. The corner-
	and anowed to reach equilibrium. Under tins load, the gauge length alongates electically by 46 mm. No solid sugar is observed within the	sharing octaneural the angles range from 19-44. De is bolided to six equivalent Be, three equivalent Mn, and three equivalent Al atoms
	container. The temperature is then lowered to a temperature T1 and	to form a mixture of edge face and corner-sharing ReMnaRe ΔI_{a}
	allowed to reach equilibrium. At temperature T1 it is observed that only	cuboctahedra. There are three shorter (2.12 Å) and three longer (2.17 Å)
	solid sugar and solid water (ice) exist. There is no solubility of sugar	Be–Be bond lengths. All Be–Mn bond lengths are 2.51 Å. All Be–Al
	in solid water, nor of water in solid sugar. How many grams of ice are	bond lengths are 2.52 Å. Mn is bonded in a 16-coordinate geometry to
	present in this container?	twelve equivalent Be and four equivalent Al atoms. All Mn-Al bond
	(a) 68 g	lengths are 2.63 Å. Al is bonded in a 16-coordinate geometry to twelve
	(b) 32 g	equivalent Be and four equivalent Mn atoms.
	(c) 36 g	
	(d) None of these options	(Note: This information is misleading rather than superfluous)

Matbench_steels dataset PCA and correlation analysis

 $PC1_Correlation = -0.145$

 $PC2_Correlation = 0.436$



MAGPIE Features used to train the RFR model

The following MAGPIE features were used to train the *RFR* model:

- Features:
 - Number, MendeleevNumber, AtomicWeight, MeltingT, Column, Row
 - CovalentRadius, Electronegativity,
 - NsValence, NpValence, NdValence, NfValence, NValence
 - NsUnfilled, NpUnfilled, NdUnfilled, NfUnfilled, NUnfilled
 - GSvolume_pa, GSbandgap, GSmagmom
- Statistical Descriptors:
 - mean, avg_dev, minimum, maximum, range

Example prompt of crystal structure descriptions from LLM-Prop band gap dataset

KPrNbMnO₆ is (Cubic) Perovskite-derived structured and crystallizes in the <mark>cubic</mark> Type F43m space group. K^{1+} is bonded to twelve equivalent O^{2-} atoms to form KO_{12} Space Group cuboctahedra that share corners with twelve equivalent KO12 cuboctahedra, faces with six equivalent PrO_{12} cuboctahedra, faces with four equivalent NbO_6 octahedra, and Coordination faces with four equivalent MnO₅ octahedra. All K-O bond lengths are 2.83 Å. Pr³+ is **Bond Angle** bonded to twelve equivalent 0^{2-} atoms to form PrO_{12} cuboctahedra that share corners with twelve equivalent PrO₁₂ cuboctahedra, faces with six equivalent KO₁₂ cuboctahedra, faces with four equivalent NbO₆ octahedra, and faces with four equivalent MnO₆ octahedra. All Pr-O bond lengths are 2.83 Å. Nb⁵⁺ is bonded to six equivalent O^{2−} atoms to form NbO₆ octahedra that share corners with six equivalent MnO_6 octahedra, faces with four equivalent KO_{12} cuboctahedra, and faces with four equivalent PrO12 cuboctahedra. The corner-sharing octahedra are not tilted. All Nb-O bond lengths are 2.00 Å. Mn³⁺ is bonded to six equivalent O²⁻ atoms to form MnO₆ octahedra that share corners with six equivalent NbO $_{6}$ octahedra, faces with four equivalent KO12 cuboctahedra, and faces with four equivalent PrO12 cuboctahedra. The corner-sharing octahedra are not tilted. All Mn–O bond lengths are 2.01 Å. 0^{2-} is bonded in a distorted linear geometry to two equivalent K¹⁺, two equivalent Pr³⁺, one Nb⁵+, and one Mn³+ atom.