Supplementary Information:A Multimodal Framework for Material Discovery: Infusing Large Language Models with Atomic Structures

Yingheng Tang[1*], Wenbin Xu[2*], Jie Cao[4], Jianzhu Ma[3], Weilu Gao[5*], Steve Farrell[2], Benjamin Erichson[6,7], Michael W. Mahoney[6,7,8], Andy Nonaka[1], Zhi Yao[1*]

[1]Applied Mathematics and Computational Research Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA.
[2]National Energy Research Scientific Computing Center, Lawrence Berkeley National Laboratory, Berkeley, CA, USA.
[3]Institute for AI Industry Research, Tsinghua University, Beijing, China.
[4]NSF National AI Institute for Student-AI Teaming, University of Colorado at Boulder, Boulder, USA.
[5]Department of Electrical and Computer Engineering, The University of Utah, Salt Lake City, UT, USA.
[6]Scientific Data Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA.
[7]International Computer Science Institute, Berkeley, CA, USA.
[8]Department of Statistics, University of California at Berkeley, Berkeley, CA, USA.

*Corresponding author(s). E-mail(s): ytang4@lbl.gov; wenbinxu@lbl.gov; weilugao@utah.edu; jackie_zhiyao@lbl.gov;

Keywords: Foundational model, Large Language Model, multi-modal learning, Material discovery

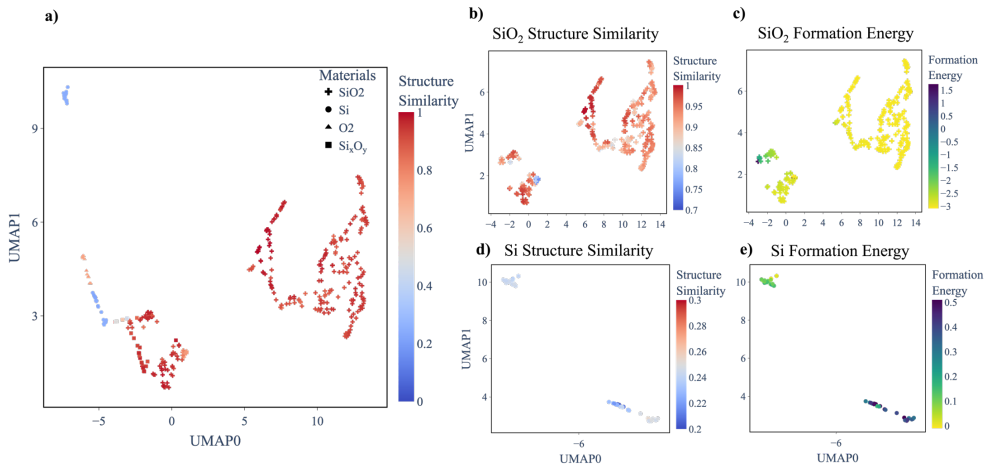

Fig. 1 UMAP visualization of structural embeddings extracted from the bridge model. (Si, O, Si_xO_y)

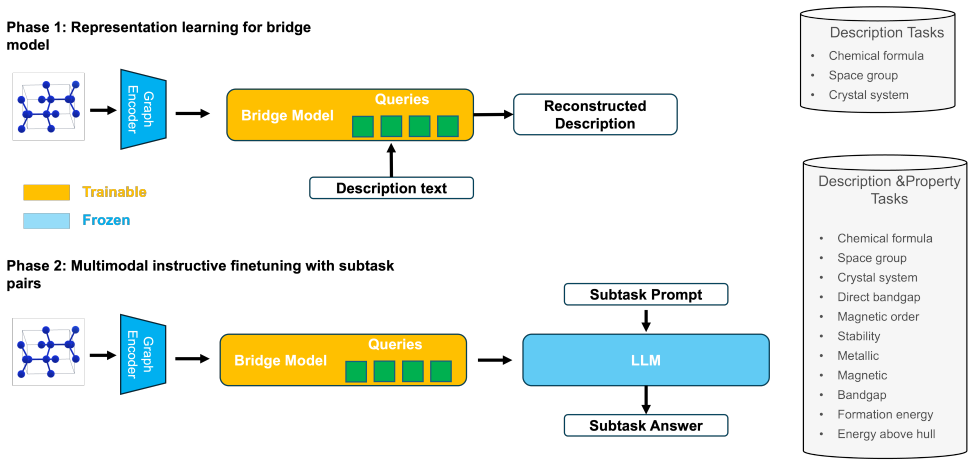

Fig. 2 Training Scheme.

Instruction Templates (descriptive tasks)

Task	Instruction Template
Reduced Formula	<material structure>What is the chemical formula for this material? <material structure>Can you tell me the chemical formula of this material? <material structure>Please provide the chemical formula for the material. <material structure>What is the formula for this material? <material structure>Could you tell me the formula of the material? <material structure>What elements make up this material? <material structure>How would you write the chemical formula of this material? <material structure>What is the exact chemical formula of this material? <material structure>Can you provide the chemical formula for this material?
Space Group	<material structure>What is the space group for this material? <material structure>To which space group does this material belong? <material structure>Can you tell me the space group of this material? <material structure>Please provide the space group for the material. <material structure>What is the crystallographic space group of this material? <material structure>How is the space group of this material classified? <material structure>Can you specify the space group for this material? <material structure>Could you tell me the space group classification of this material? <material structure>Can you provide the space group information for this material? <material structure>What is the space group number of this material?
Crystal System	<material structure>What is the crystal system of this material? <material structure>Can you tell me the crystal system of this material? <material structure>Please provide the crystal system for the material. <material structure>What crystal system does this material belong to? <material structure>How is the crystal system of this material classified? <material structure>Can you specify the crystal system for this material? <material structure>What is the crystallographic system of this material? <material structure>Could you tell me the crystal system classification of this material? <material structure>Which crystallographic system does this material belong to?
Generate	<material structure>Can you provide another material similar to this material? <material structure>Is there another material like this material that you can provide? <material structure>Can you show me a different material similar to this one? <material structure>Can you generate another material similar to this one?
General	<material structure>Can you describe this material? <material structure><s>

Answer Templates (descriptive tasks)

Task	Instruction Template
Reduced Formula	The chemical formula for this material is <material attribute >. The chemical formula of this material is <material attribute >. The chemical formula for the material is <material attribute >. The formula for this material is <material attribute >. The formula of the material is <material attribute >. The elements that make up this material are represented as <material attribute >. The chemical formula of this material is written as <material attribute >. The exact chemical formula of this material is <material attribute >. The chemical formula for this material is <material attribute >.
Space Group	The space group for this material is <material attribute >. This material belongs to the space group <material attribute >. The space group of this material is <material attribute >. The space group for the material is <material attribute >. The crystallographic space group of this material is <material attribute >. The space group of this material is classified as <material attribute >. The space group for this material is specified as <material attribute >. The space group classification of this material is <material attribute >. The space group information for this material is <material attribute >. The space group number of this material is <material attribute >.
Crystal System	The crystal system of this material is <material attribute >. The crystal system of this material is <material attribute >. The crystal system for the material is <material attribute >. This material belongs to the <material attribute >crystal system. The crystal system of this material is classified as <material attribute >. The crystal system for this material is specified as <material attribute >. The crystallographic system of this material is <material attribute >. The crystal system classification of this material is <material attribute >. This material belongs to the <material attribute >crystallographic system.

Instruction Templates (property part1)

Task	Instruction Template
Is Metal	<material structure>Is this material metal or non-metal?
	<material structure>Can you tell me if this material is metal or not?
	<material structure>What is the classification of this material: metal or non-metal?
	<material structure>Is this material considered a metal?
	<material structure>How is this material categorized: metal or non-metal?
	<material structure>Could you specify if this material is metal or non-metal?
	<material structure>Is the material metallic or non-metallic?
	<material structure>Can you provide the classification of this material: metal or non-metal?
	<material structure>Is this material identified as a metal or non-metal?
	<material structure>What type of material is this: metal or non-metal?
Direct Bandgap	<material structure>Does the material have a direct bandgap or indirect bandgap?
	<material structure>Is the bandgap of this material direct or indirect?
	<material structure>Can you tell me if this material has a direct or indirect bandgap?
	<material structure>What type of bandgap does this material have: direct or indirect?
	<material structure>Is this material characterized by a direct or indirect bandgap?
	<material structure>Could you specify if the bandgap of this material is direct or indirect?
	<material structure>Does this material exhibit a direct or indirect bandgap?
	<material structure>Is the bandgap in this material direct or indirect?
	<material structure>How is the bandgap of this material classified: direct or indirect?
	<material structure>Is this a direct or indirect bandgap material?
Stability	<material structure>Is this material stable?
	<material structure>Can you tell me if this material is stable?
	<material structure>What is the stability of this material?
	<material structure>Please provide the stability information for this material.
	<material structure>Is the material stable under standard conditions?
	<material structure>Is this material thermodynamically stable?
Experimental Observation	<material structure>Is the material experimentally observed or not?
	<material structure>Can you tell me if the material is observed in experiments?
Is Magnetic	<material structure>Is the material magnetic or not?
	<material structure>Is the material magnetic or non-magnetic?
	<material structure>Can you tell me if this material is magnetic?
	<material structure>What is the magnetic nature of this material?
	<material structure>Is this material classified as magnetic?
	<material structure>Does this material have magnetic properties?
	<material structure>Is this a magnetic or non-magnetic material?
Magnetic Order	<material structure>What is the magnetic order of the material?
	<material structure>Can you tell me the magnetic order of this material?
	<material structure>Could you specify the magnetic order of the material?
	<material structure>What type of magnetic order does this material have?
	<material structure>Please provide the magnetic ordering of the material.
	<material structure>What is the magnetic arrangement in this material?
	<material structure>Could you tell me the type of magnetic order of this material?

Answer Templates (property part1)

Task	Instruction Template
Is Metal	This material is classified as <material attribute >. This material is a <material attribute >. The classification of this material is <material attribute >. This material is considered <material attribute >. This material is categorized as <material attribute >. This material is specified as <material attribute >. This material is <material attribute >. The classification of this material is <material attribute >. This material is identified as <material attribute >. This type of material is <material attribute >.
Direct Bandgap	The material has a <material attribute >bandgap. The bandgap of this material is <material attribute >. This material has a <material attribute >bandgap. This material has a <material attribute >type of bandgap. This material is characterized by a <material attribute >bandgap. The bandgap of this material is specified as <material attribute >. This material exhibits a <material attribute >bandgap. The bandgap in this material is <material attribute >. The bandgap of this material is classified as <material attribute >. This is a <material attribute >bandgap material.
Stability	This material is <material attribute >. Yes, this material is <material attribute >. The stability of this material is <material attribute >. The stability information for this material is <material attribute >. This material is <material attribute >under standard conditions. This material is <material attribute >.
Experimental Observation	The material is <material attribute >. The material is <material attribute >.
Is Magnetic	The material is <material attribute >. This material is <material attribute >. Yes, this material is <material attribute >. The magnetic nature of this material is <material attribute >. This material is classified as <material attribute >. This material has <material attribute >properties. This is a <material attribute >material.
Magnetic Order	The magnetic order of the material is <material attribute >. The magnetic order of this material is <material attribute >. The magnetic order of the material is specified as <material attribute >. This material has a <material attribute >type of magnetic order. The magnetic ordering of the material is <material attribute >. The magnetic arrangement in this material is <material attribute >. The type of magnetic order of this material is <material attribute >.

Instruction Templates (property part2)

Task	Instruction Template
Bandgap	<material structure>What is the bandgap of the material?
	<material structure>Can you tell me the bandgap of this material?
	<material structure>What is the energy bandgap for this material?
	<material structure>Could you specify the bandgap of the material?
	<material structure>Could you tell me the bandgap energy level of this material?
Formation Energy	<material structure>Can you tell me the formation energy of this material?
	<material structure>Please provide the formation energy for the material.
	<material structure>What is the formation energy value for this material?
	<material structure>How much is the formation energy of this material?
	<material structure>Can you specify the formation energy of this material?
Energy Above Hull	<material structure>Can you tell me the energy above hull of this material?
	<material structure>Please provide the energy above hull for the material.
	<material structure>What is the energy above the hull for this material?
	<material structure>How much is the energy above hull for this material?
	<material structure>Can you specify the energy above hull of this material?
	<material structure>Could you tell me the energy above hull of the material?

Answer Templates (property part2)

Task	Instruction Template
Bandgap	The bandgap of the material is <material attribute >. The bandgap of this material is <material attribute >. The energy bandgap for this material is <material attribute >. The bandgap of the material is specified as <material attribute >. The bandgap energy level of this material is <material attribute >.
Formation Energy	The formation energy of this material is <material attribute >. The formation energy for the material is <material attribute >. The formation energy value for this material is <material attribute >. The formation energy of this material is <material attribute >. The formation energy of this material is specified as <material attribute >.
Energy Above Hull	The energy above hull of this material is <material attribute >. The energy above hull for the material is <material attribute >. The energy above the hull for this material is <material attribute >. The energy above hull for this material is <material attribute >. The energy above hull of this material is specified as <material attribute >. The energy above hull of the material is <material attribute >.