Supplementary Information: MatterChat: A Multi-Modal LLM for Material Science

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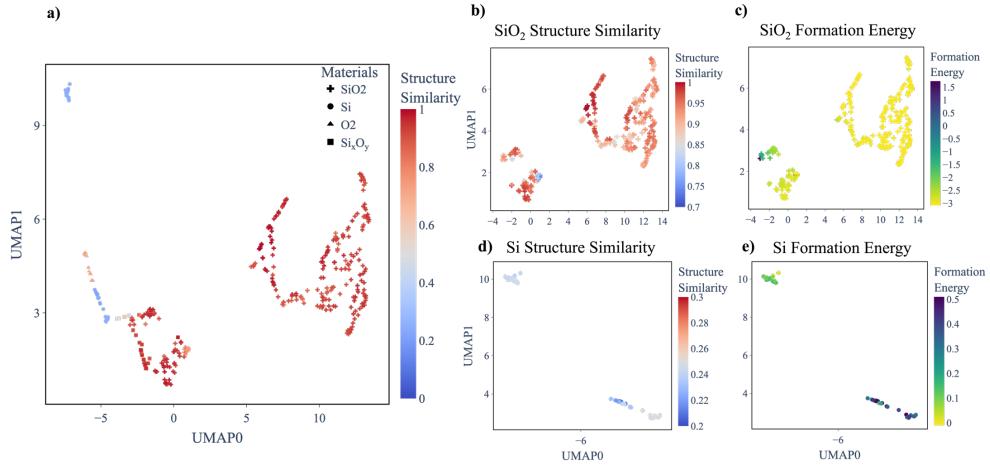[6]International Computer Science Institute, Berkeley, CA, USA.
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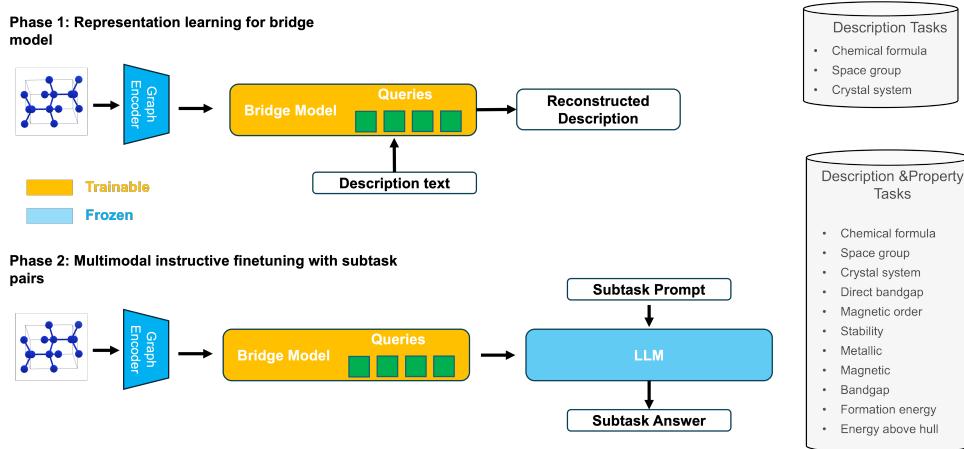[†]These authors contribute equally

1

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

Phase 1: Representation learning for bridge model

Trainable

Frozen

Queries

Bridge Model

Graph Encoder

Description text

Reconstructed Description

Phase 2: Multimodal instructive finetuning with subtask pairs

Graph Encoder

Bridge Model

Queries

Subtask Prompt

LLM

Subtask Answer

Description Tasks
- Chemical formula
- Space group
- Crystal system

Description &Property Tasks
- Chemical formula
- Space group
- Crystal system
- Direct bandgap
- Magnetic order
- Stability
- Metallic
- Magnetic
- Bandgap
- Formation energy
- Energy above hull

Fig. 2 Training Scheme.

3

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 >.