Quantitative Assessment of Crystal Structure Prediction

OPAL-Bench: an Orientation-invariant, Polymorph-Aware, Large Benchmark

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Juanita Puentes Nicolás Aparicio Paula Cárdenas Pablo Arbeláez

Universidad de los Andes, Colombia · *Equal contribution

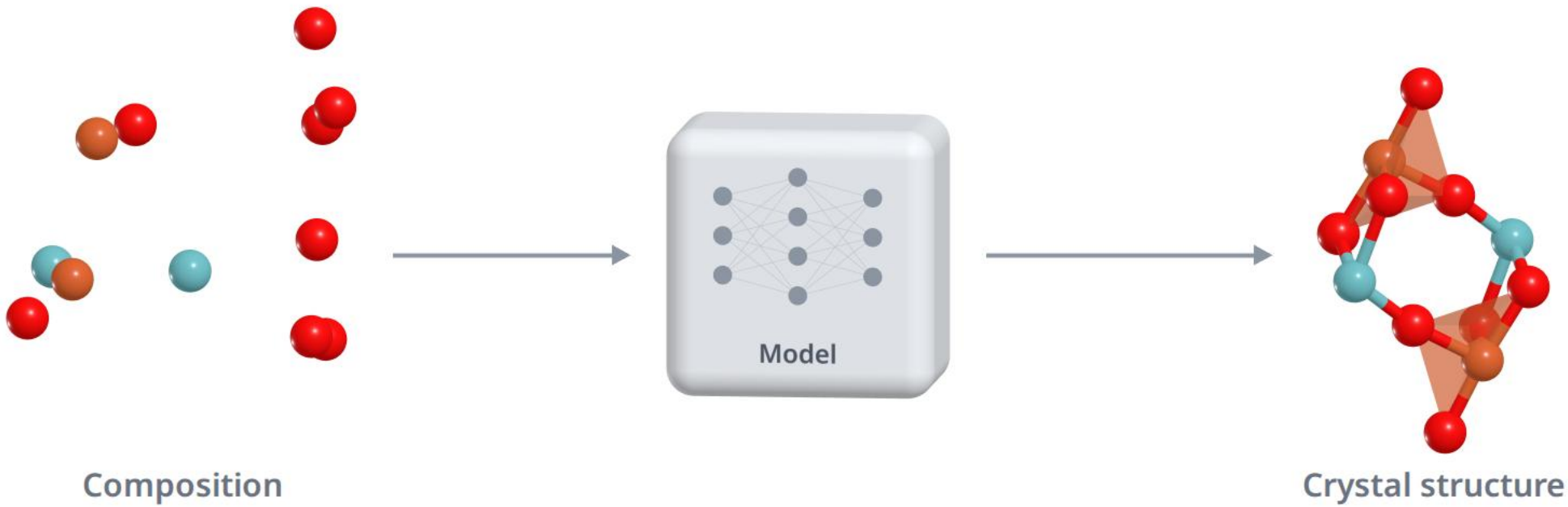
NeurIPS 2026 · Evaluations and Datasets Track

Universidad de los Andes Colombia | BIOMEDICAL COMPUTER VISION

NEURAL INFORMATION PROCESSING SYSTEMS

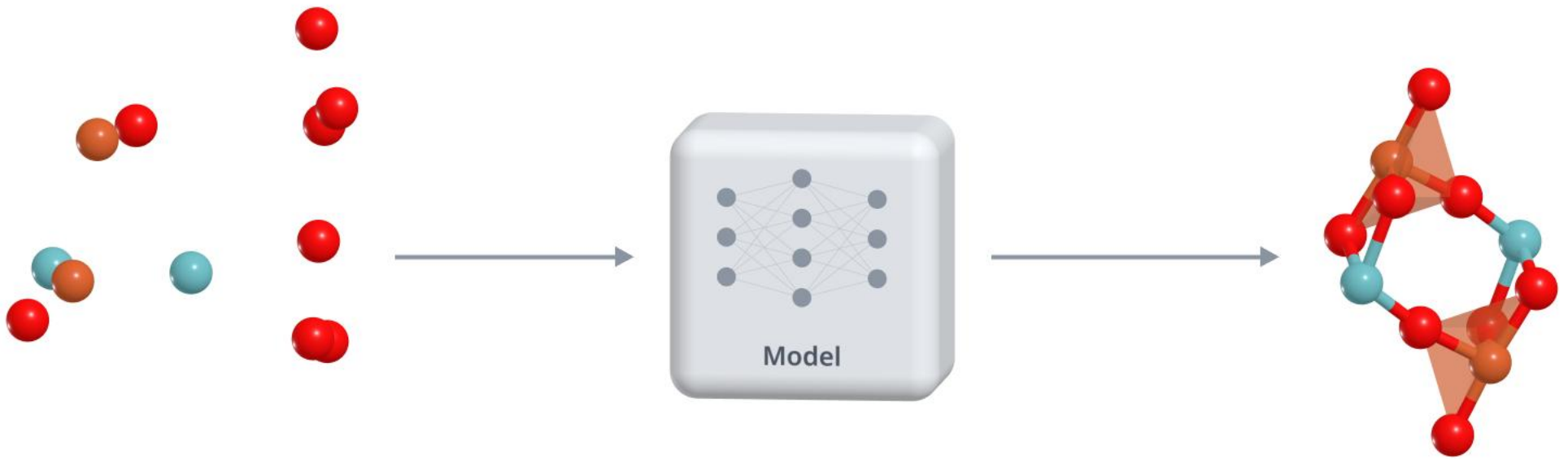
Crystal Structure Prediction (CSP)

Predict how atoms arrange in a crystal from its composition alone



Crystal Structure Prediction (CSP)

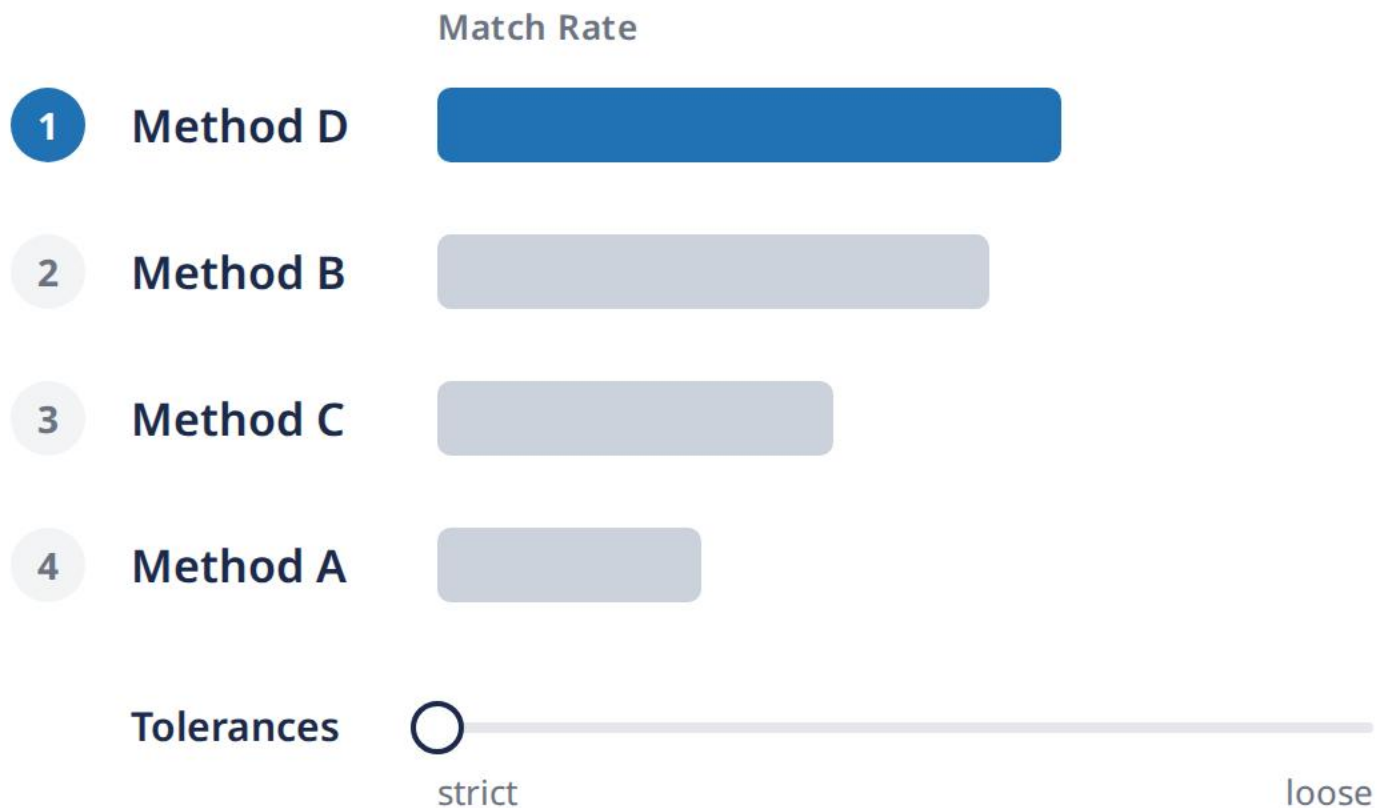
Predict how atoms arrange in a crystal from its composition alone



Generative models keep improving,
but we identify *key issues in how they are evaluated*

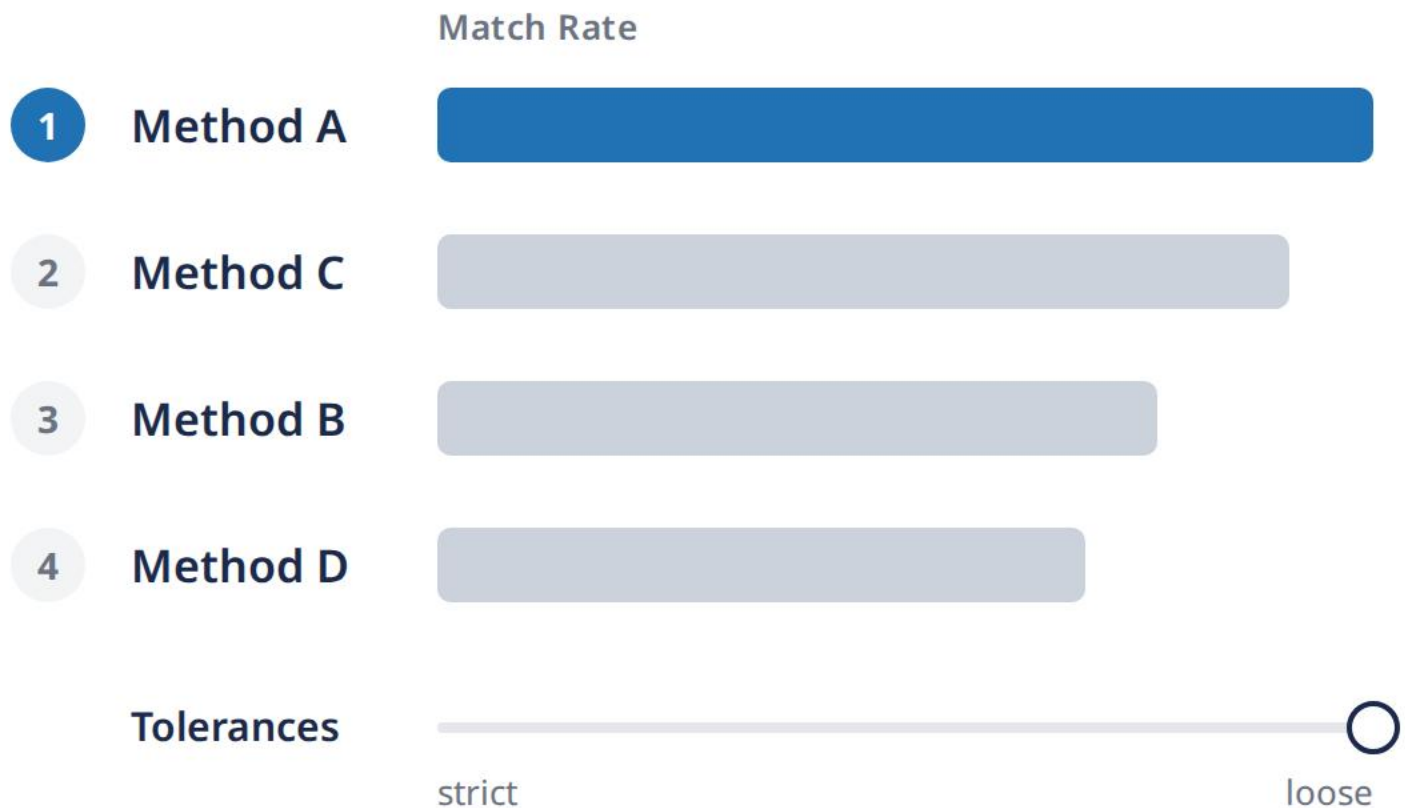
CSP EVALUATION · PROBLEM 1

Tolerance-dependent scores



CSP EVALUATION · PROBLEM 1

Tolerance-dependent scores



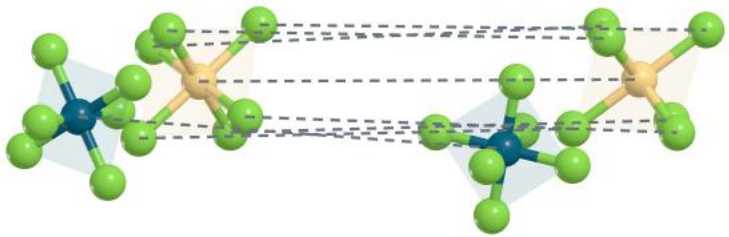
We find that method rankings are sensitive to the chosen tolerance

OPAL-BENCH · SOLUTION

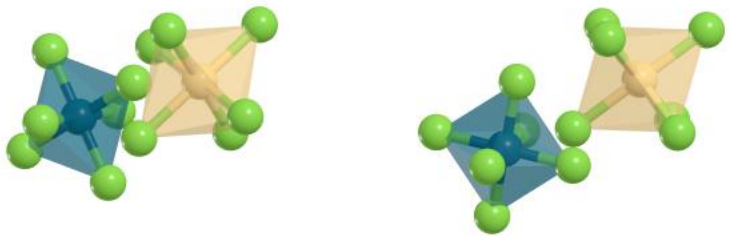
Tolerance-free distances

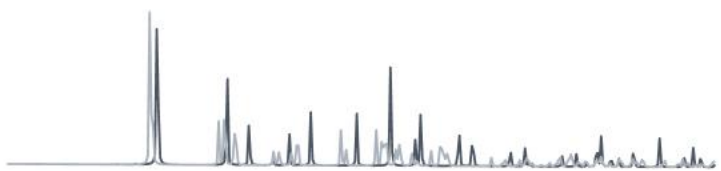
4 geometric and 5 physical distance metrics

Geometric



Physical



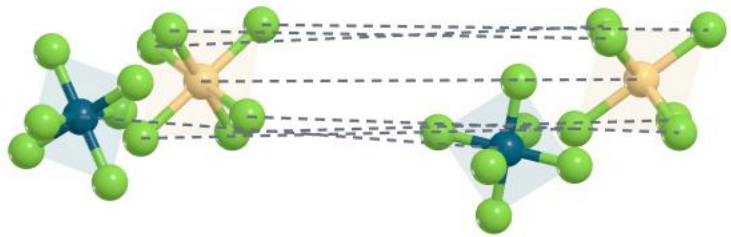


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Tolerance-free distances

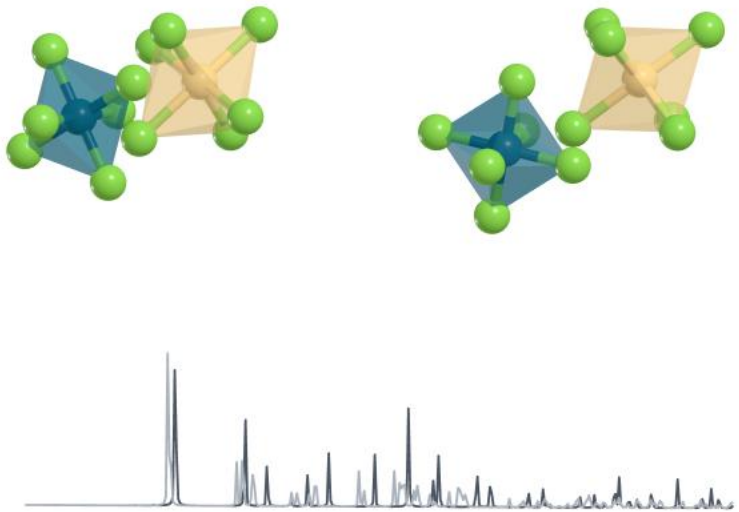
4 geometric and 5 physical distance metrics

Geometric



Chamfer · Hausdorff · Sinkhorn · RMSE

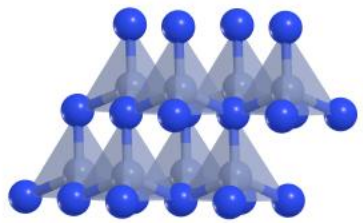
Physical



Density · SOAP · XRD · Formation energy · Relaxed formation energy

CSP EVALUATION · PROBLEM 2

Polymorphs are ignored

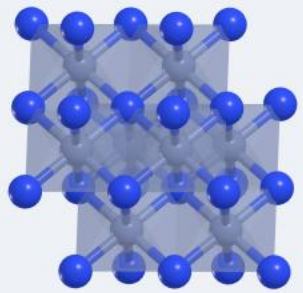


Prediction

CrN



distance

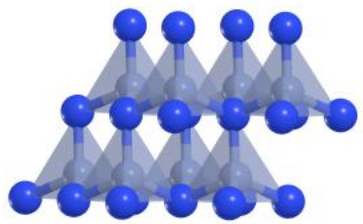


Single reference

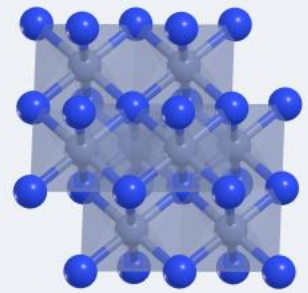
another CrN polymorph

CSP EVALUATION · PROBLEM 2

Polymorphs are ignored



distance



Prediction
CrN

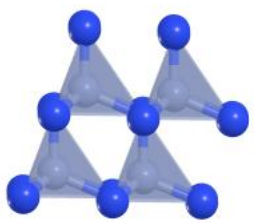
Single reference
another CrN polymorph

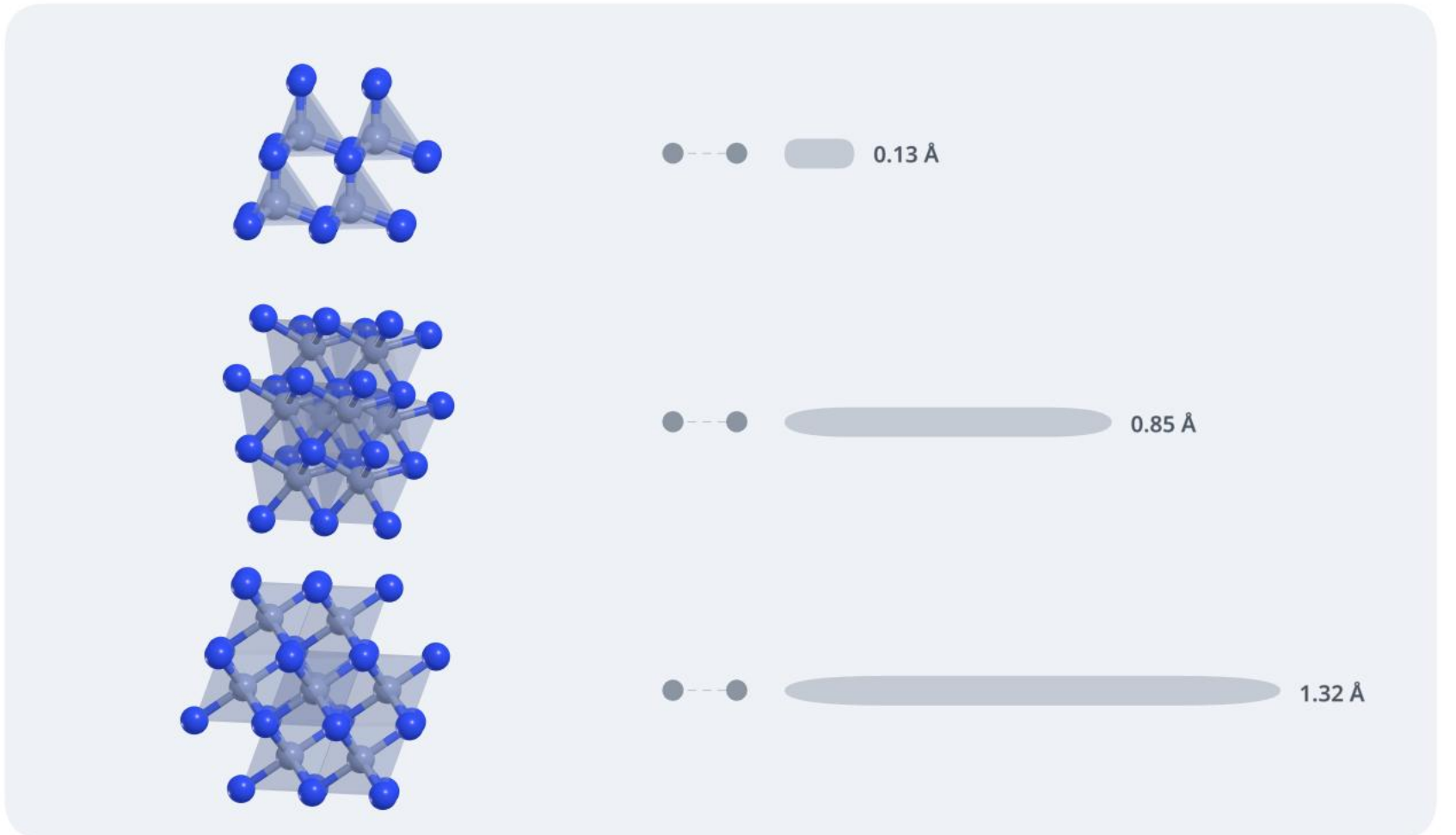
A composition can crystallize in several stable structures, but only one is used as reference

OPAL-BENCH · SOLUTION

Compare against all known polymorphs

Each metric scores its own closest known polymorph

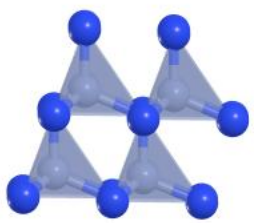


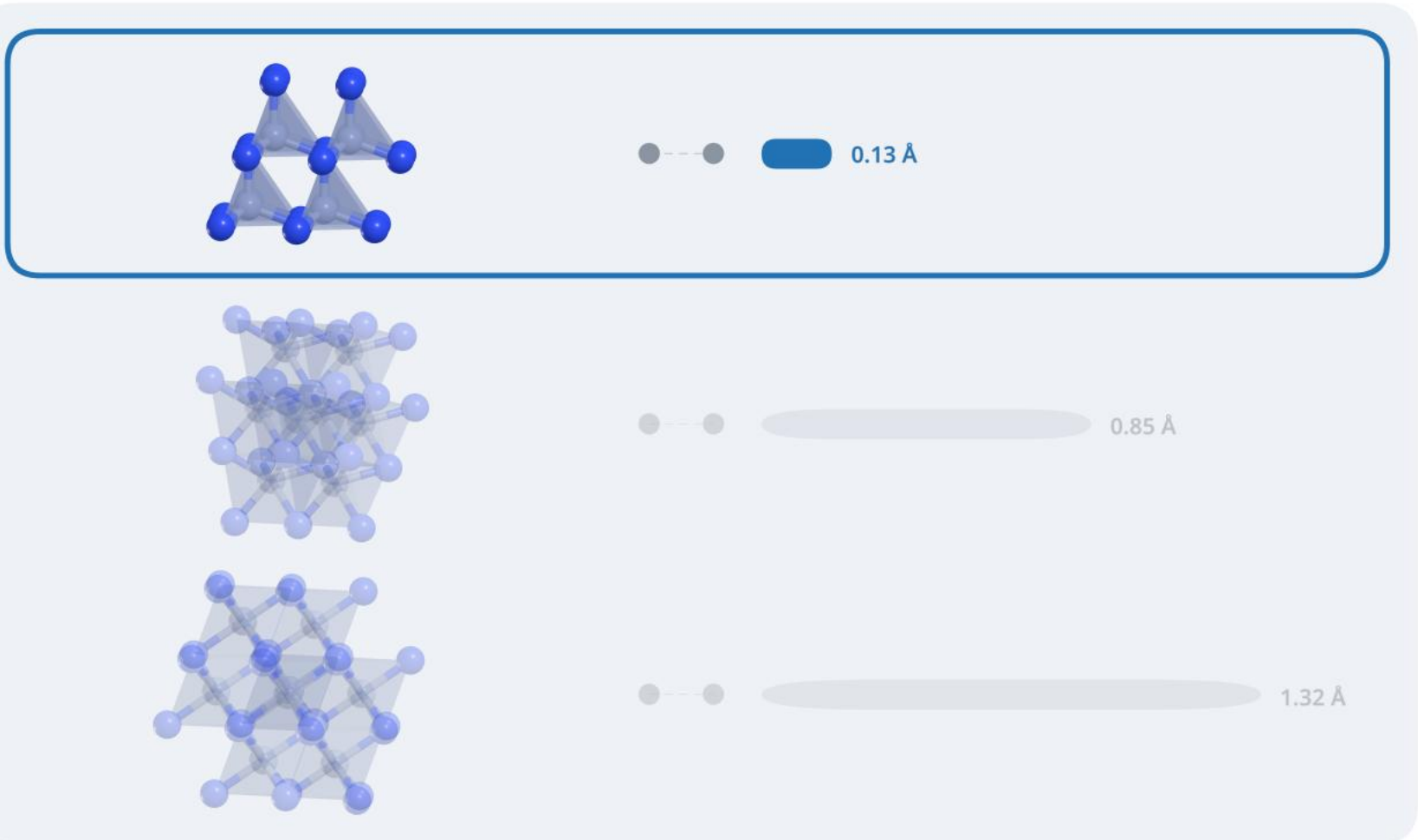


OPAL-BENCH · SOLUTION

Compare against all known polymorphs

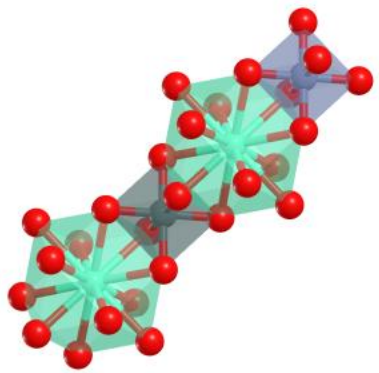
Each metric scores its own closest known polymorph





CSP EVALUATION · PROBLEM 3

Distances depend on orientation

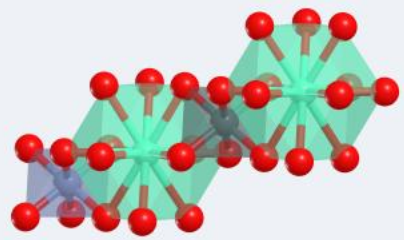


Prediction

same crystal, rotated



distance

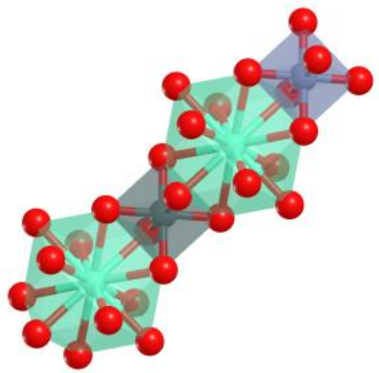


Reference

Eu_2CrSnO_6

CSP EVALUATION · PROBLEM 3

Distances depend on orientation

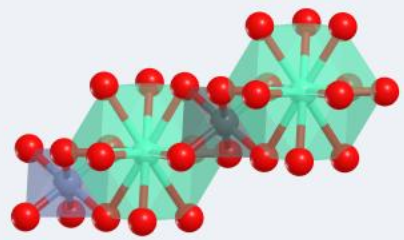


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Reference

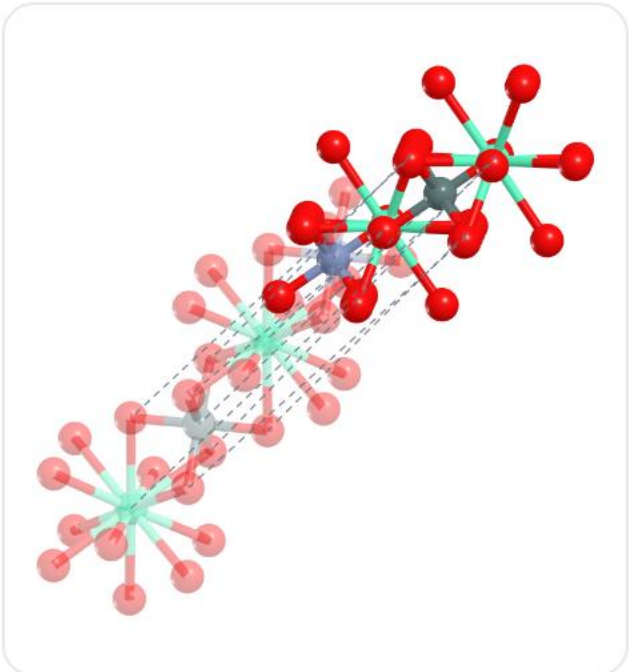
Eu_2CrSnO_6

Without alignment, rotations and atom ordering inflate the distance

OPAL-BENCH · SOLUTION

Species-aware alignment

Rotation, translation and atom matching



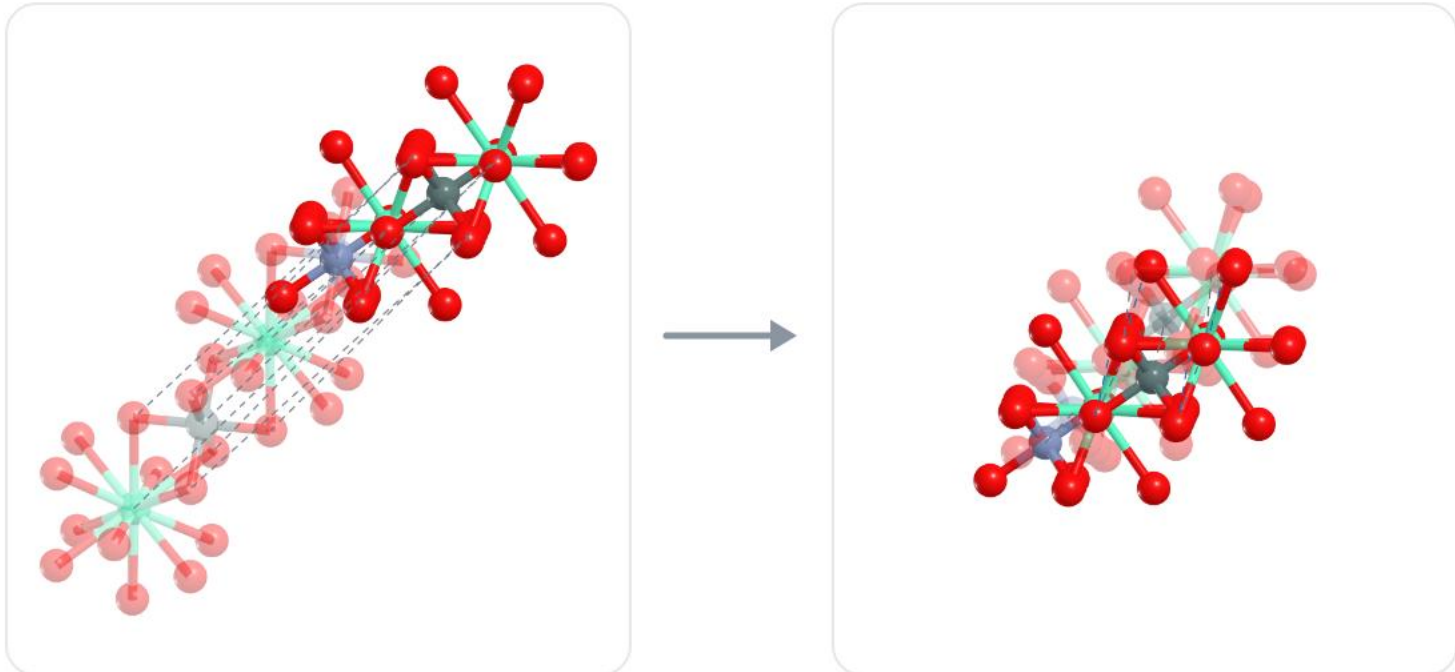
Random start

12.95 Å

OPAL-BENCH · SOLUTION

Species-aware alignment

Rotation, translation and atom matching



Random start

12.95 Å

Match atoms, rotate and translate

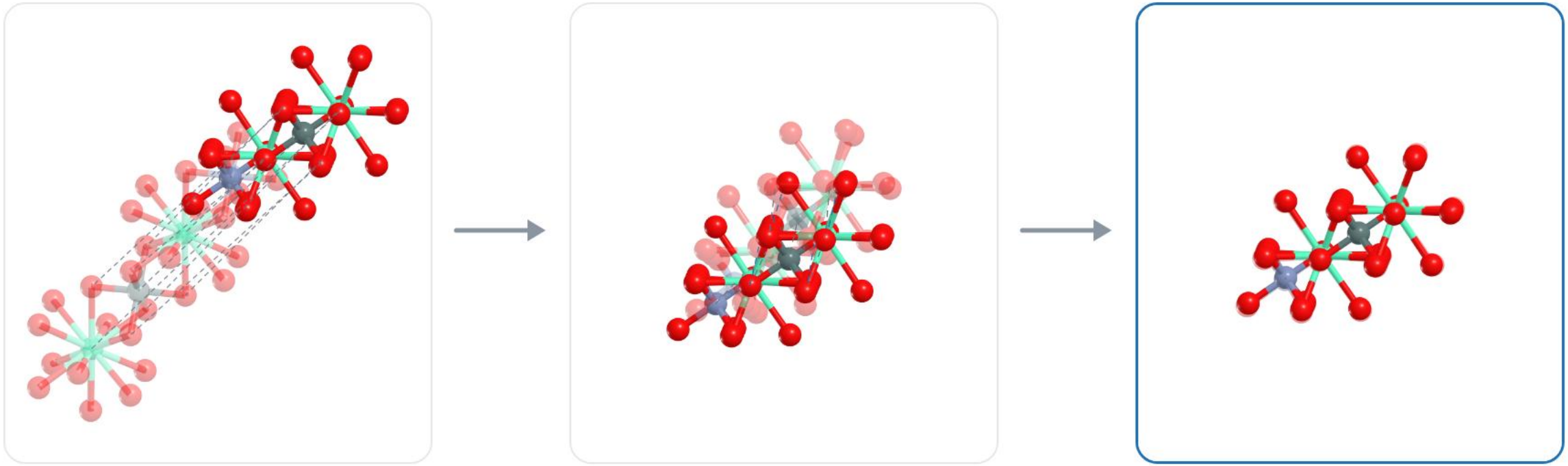
1.82 Å

Repeated until the distance stops decreasing

OPAL-BENCH · SOLUTION

Species-aware alignment

Rotation, translation and atom matching



Random start
12.95 Å

Match atoms, rotate and translate
1.82 Å

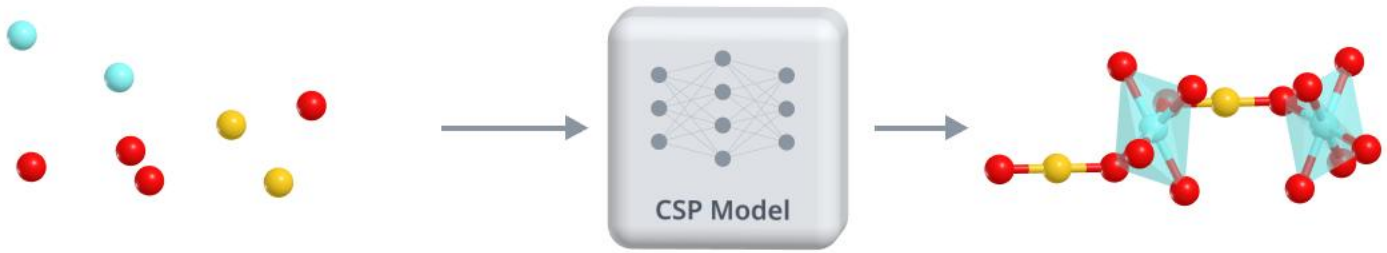
Aligned
0.064 Å

Repeated until the distance stops decreasing

OPAL-BENCH

Two tasks, two tracks

7 CSP and 2 SICSP methods, retrained from scratch on four datasets



CSP composition only

CDVAE · DiffCSP · FlowMM · FlowLLM · CrystalFlow · MatterGen · OPAL-CSP (ours)



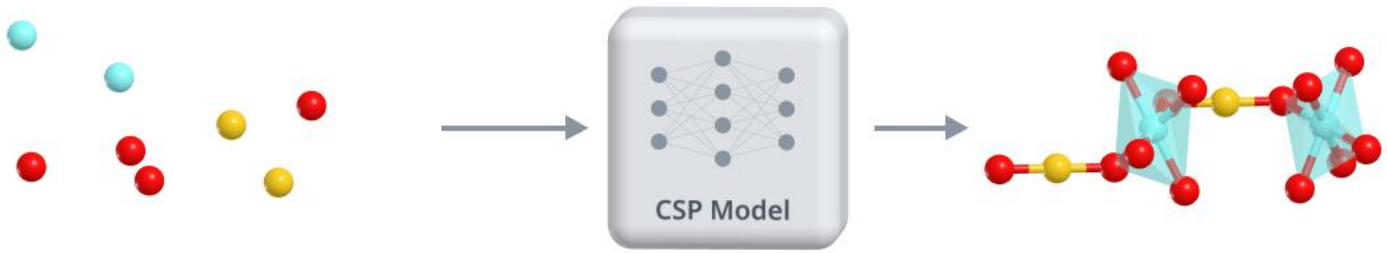
SICSP composition + symmetry

DiffCSP++ · SGEquiDiff

OPAL-BENCH

Two tasks, two tracks

7 CSP and 2 SICSP methods, retrained from scratch on four datasets



CSP composition only

CDVAE · DiffCSP · FlowMM · FlowLLM · CrystalFlow · MatterGen · OPAL-CSP (ours)



SICSP composition + symmetry

DiffCSP++ · SGEquiDiff

Templates restrict the search space,
so the two tasks are not fairly comparable and are ranked separately

OPAL-BENCH

Key findings

- **No method dominates**, and rankings shift across metrics and datasets

OPAL-BENCH

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- **Geometric and physical metrics are weakly correlated**

OPAL-BENCH

Key findings

- **No method dominates**, and rankings shift across metrics and datasets
- **Geometric and physical metrics are weakly correlated**
- **Evaluation choices matter:** with alignment and polymorph handling, scores reflect structural differences instead of evaluation artifacts

Thank you

Come see us at our poster in Sydney!

Paper	arxiv.org/abs/2611.10380
Code	github.com/BCV-Uniandes/OPAL
Project page	bcv-uniandes.github.io/OPAL-WP



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