Natural Language to SQL

AiiDA Query Analysis Report

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AiiDA Natural Language Query Demo

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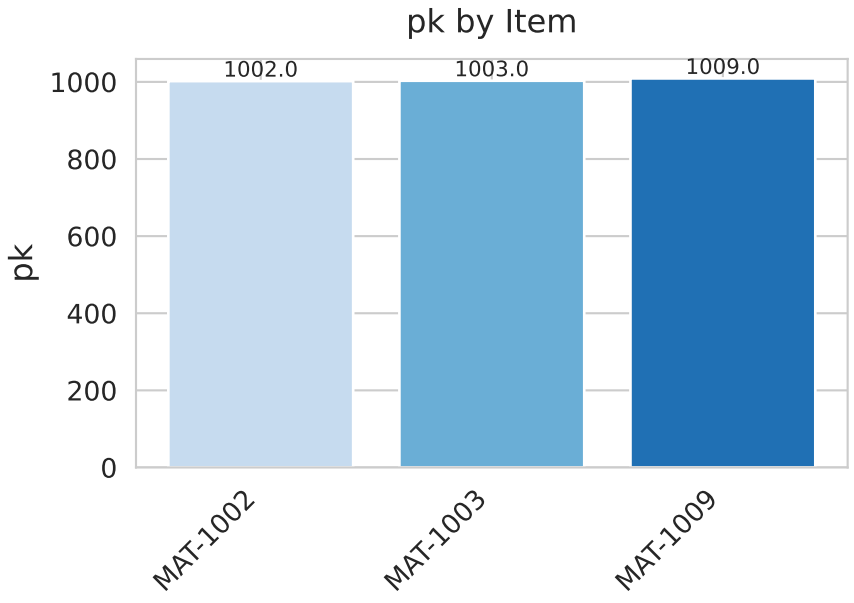
Query 1 Results: Materials Domain

Natural language: 'Find all crystal structures with bandgap greater than 2 eV and containing silicon'

Query Results

id	pk	formula	elements	crystal_system	bandgap	formation_energy
MAT-1002	1002	SiO2	['Si', 'O']	hexagonal	9.0	-5.99
MAT-1003	1003	SiC	['Si', 'C']	cubic	3.2	-6.34
MAT-1009	1009	Si3N4	['Si', 'N']	hexagonal	5.3	-7.56



Data Insights

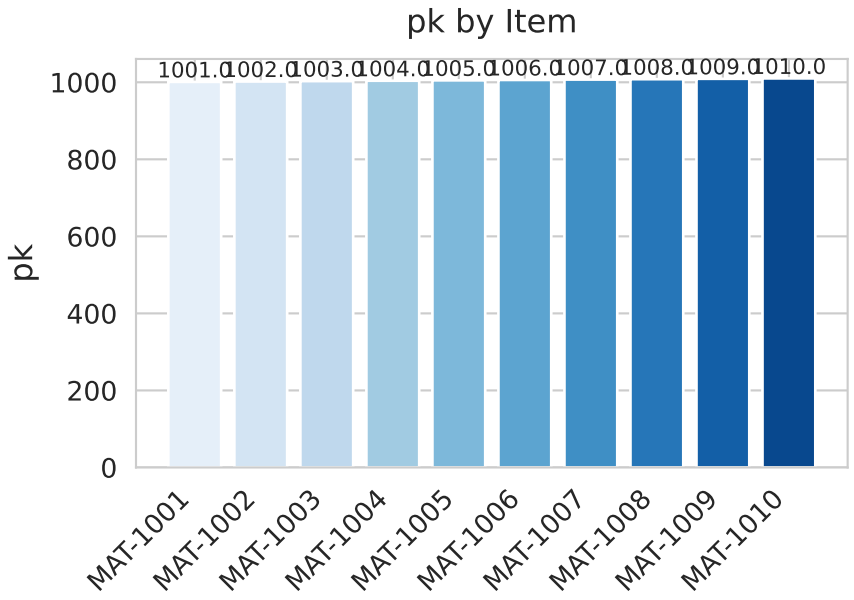
Found 3 matching records.
Average pk: 1004.67
Range of pk: 1002.00 to 1009.00
Average bandgap: 5.83
Range of bandgap: 3.20 to 9.00
Most common formula: SiO2 (1 occurrences)
1/3 materials are semiconductors.
3/3 materials contain silicon.

Query 2 Results: Materials Domain

Natural language: 'Show me density functional theory calculations for magnetic materials'

Query Results

id	pk	formula	elements	crystal_system	bandgap	formation_energy
MAT-1001	1001	Si	['Si']	cubic	1.1	-4.63
MAT-1002	1002	SiO2	['Si', 'O']	hexagonal	9.0	-5.99
MAT-1003	1003	SiC	['Si', 'C']	cubic	3.2	-6.34
MAT-1004	1004	Fe2O3	['Fe', 'O']	trigonal	2.2	-3.76
MAT-1005	1005	ZnO	['Zn', 'O']	hexagonal	3.3	-3.63



Data Insights

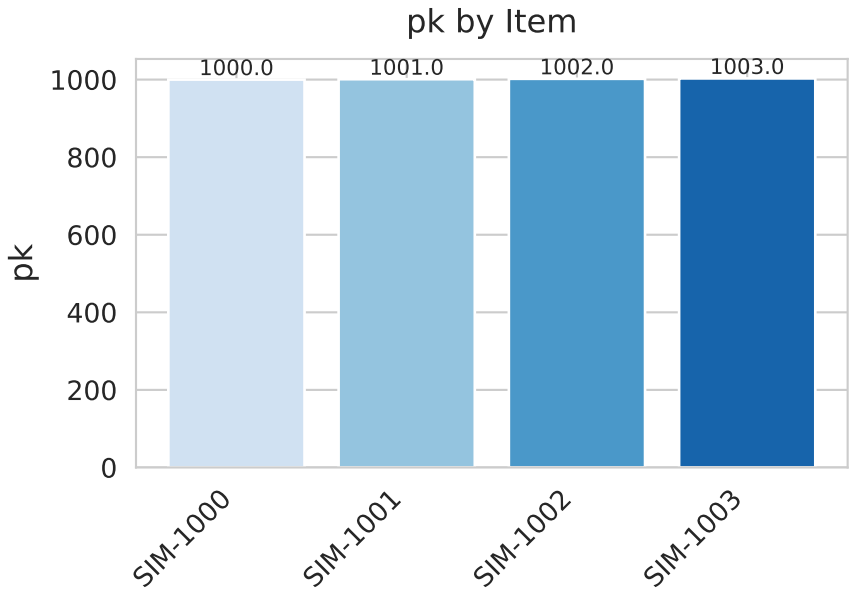
Found 10 matching records.
Average pk: 1005.50
Range of pk: 1001.00 to 1010.00
Average bandgap: 3.40
Range of bandgap: 1.10 to 9.00
Most common formula: Si (1 occurrences)
8/10 materials are semiconductors.
4/10 materials contain silicon.

Query 3 Results: Simulation Domain

Natural language: 'I need molecular dynamics simulations of water molecules at high pressure'

Query Results

id	pk	process_label	atoms	temperature	pressure	simulation_time
SIM-1000	1000	MolecularDyn	1524	724.9	57.82	56.81
SIM-1001	1001	DFTCalculati	1883	974.0	27.28	6.92
SIM-1002	1002	DFTCalculati	2141	372.7	28.79	9.49
SIM-1003	1003	MolecularDyn	4883	198.1	39.03	82.68



Data Insights

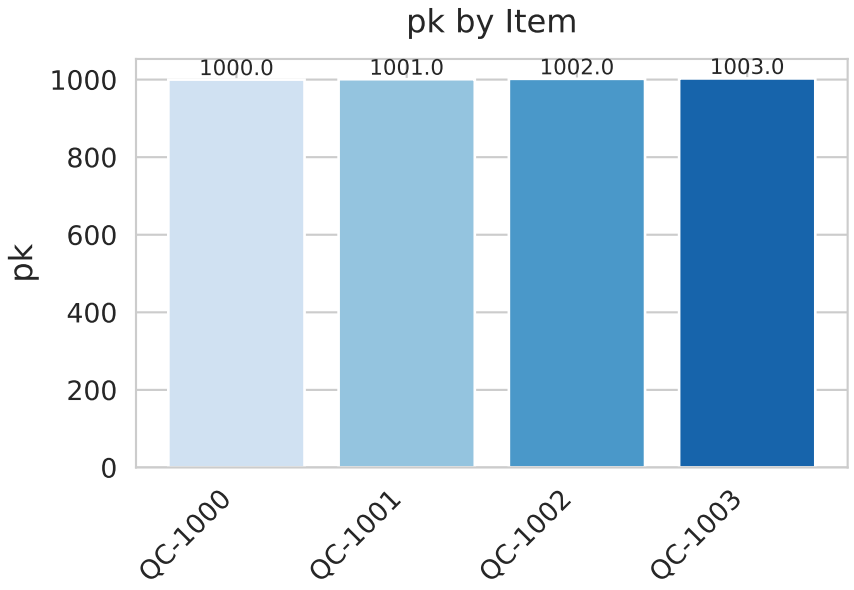
Found 4 matching records.
Average pk: 1001.50
Range of pk: 1000.00 to 1003.00
Average atoms: 2607.75
Range of atoms: 1524.00 to 4883.00
Most common process_label: MolecularDynamics (2 occurrences)
1/4 simulations at high pressure and temperature.

Query 4 Results: Quantum Domain

Natural language: 'Get quantum calculations with coherence time greater than 100 microseconds'

Query Results

id	pk	process_label	qubits	coherence	error_rate
QC-1000	1000	QubitSimulat	38	171.3	0.069
QC-1001	1001	QuantumCircu	24	184.6	0.0492
QC-1002	1002	QubitSimulat	38	57.0	0.0558
QC-1003	1003	QubitSimulat	47	15.3	0.0063



Data Insights

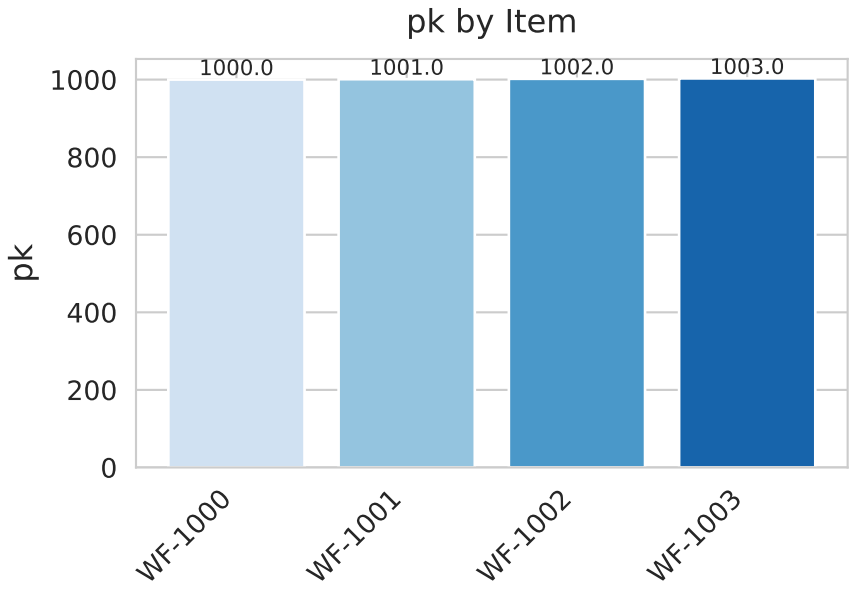
Found 4 matching records.
Average pk: 1001.50
Range of pk: 1000.00 to 1003.00
Average qubits: 36.75
Range of qubits: 24.00 to 47.00
Most common process_label: QubitSimulation (3 occurrences)
Median coherence time: 114.15

Query 5 Results: Workflow Domain

Natural language: 'Find workflows that process crystal structures and run DFT calculations'

Query Results

id	pk	process_label	state	ctime
WF-1000	1000	RelaxationWo	finished	2023-05-24
WF-1001	1001	RelaxationWo	running	2023-10-21
WF-1002	1002	DFTWorkflow	running	2023-07-06
WF-1003	1003	RelaxationWo	finished	2023-04-25



Data Insights

Found 4 matching records.

Average pk: 1001.50

Range of pk: 1000.00 to 1003.00

Most common process_label: RelaxationWorkflow (3 occurrence