

Fig. 1

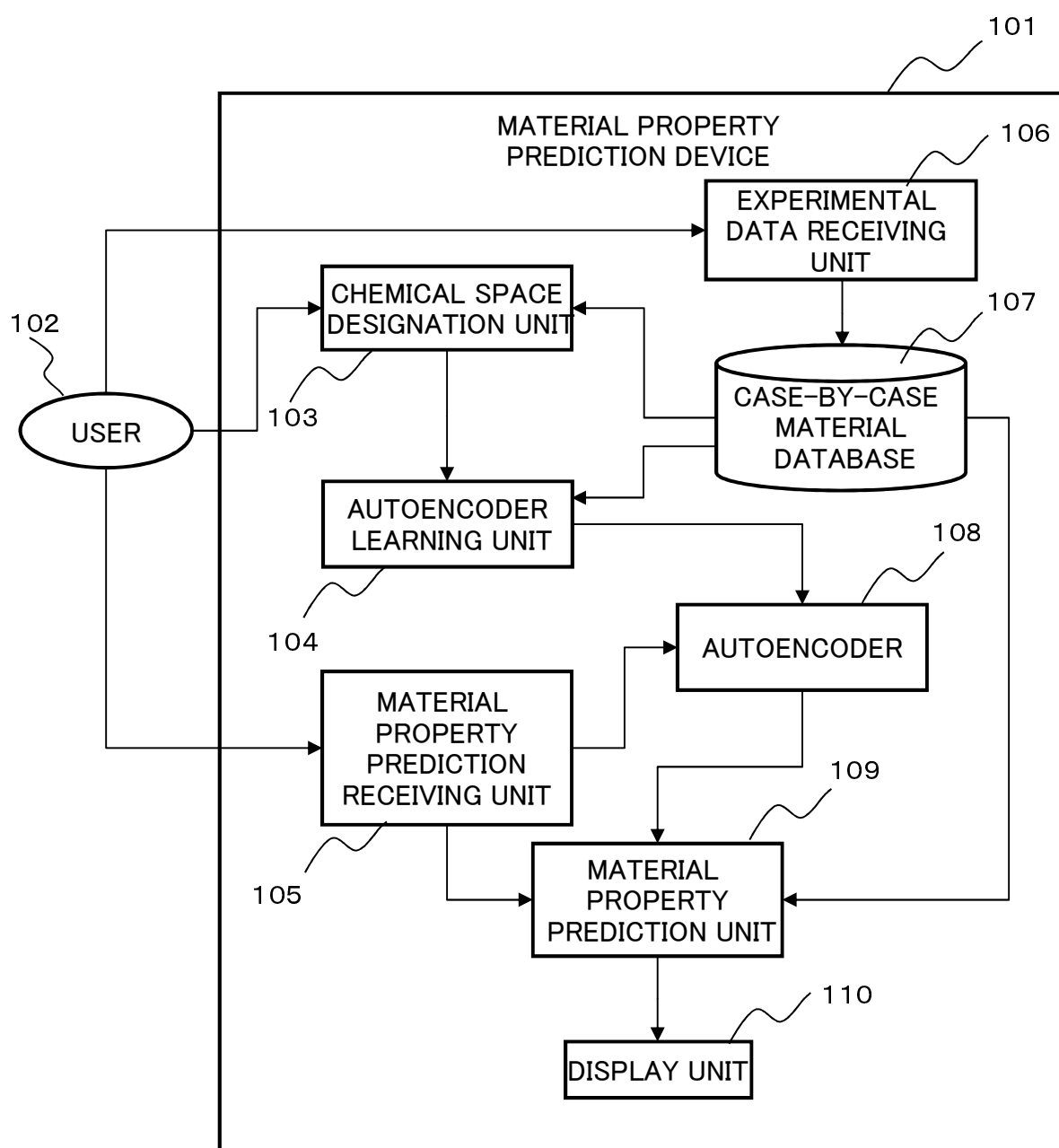


Fig. 2

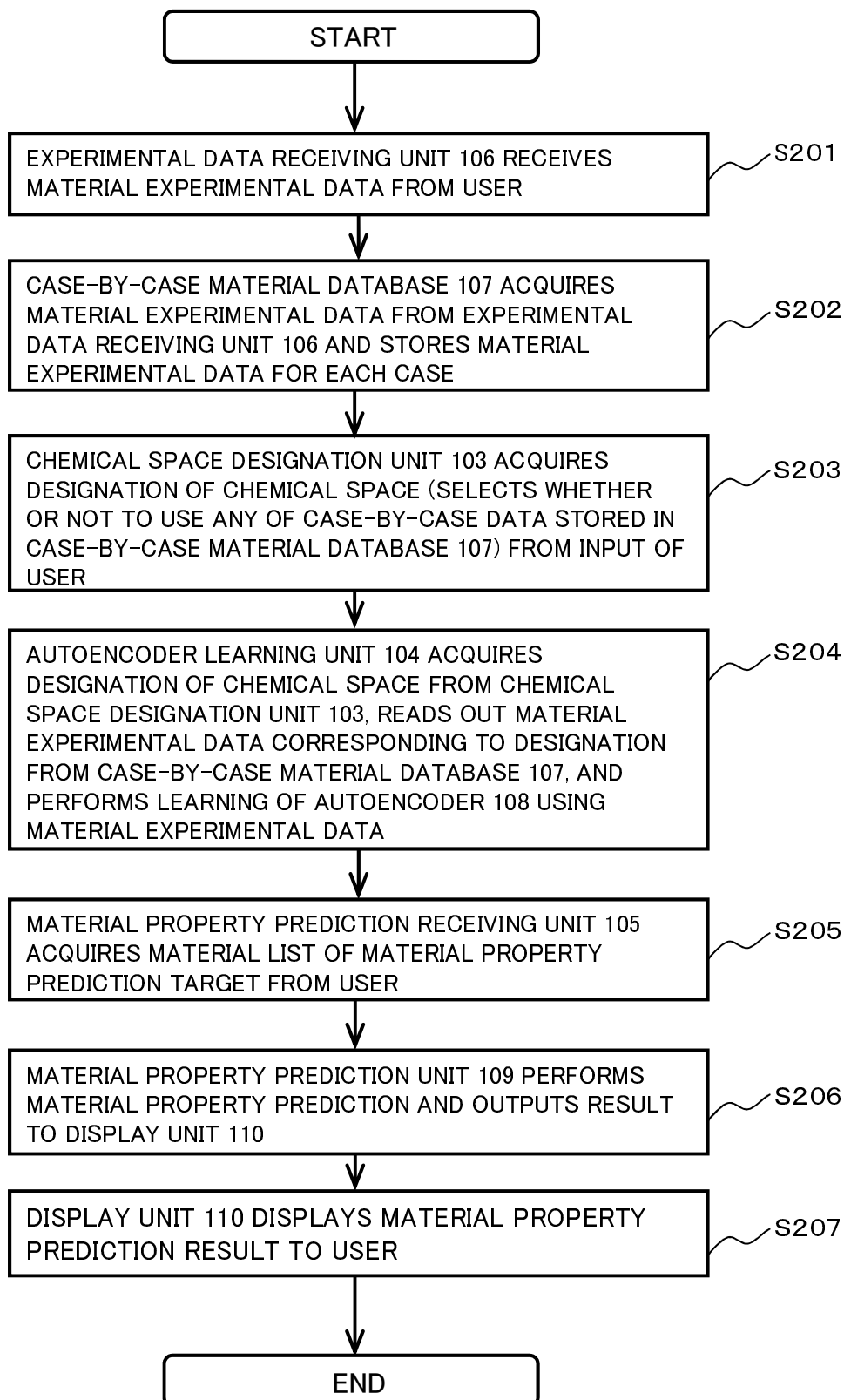


Fig. 3

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MATERIAL EXPERIMENTAL DATA HAS BEEN UPLOADED.

FILE:

BROWSE

OK

CANCEL

Fig. 4

CASE 1					
SERIAL No	STRUCTURAL FORMULA (SMILES)	EXPERIMENT CONDITION 1	EXPERIMENT CONDITION 2	MATERIAL PROPERTIES1	MATERIAL PROPERTIES2
1	<chem>CO[Si](C)(OC)N1CCCCC1</chem>	0.785	44.2	4.12	-12.5
2	<chem>CCN(CC)[Si](C)(OC)OC</chem>	0.914	35.9	1.56	29.1
3	<chem>O=C1C=CC(=O)C=C1</chem>	0.258	16.8	-0.374	35.5
⋮	⋮	⋮	⋮	⋮	⋮
CASE 2					
SERIAL No	STRUCTURAL FORMULA (SMILES)	EXPERIMENT CONDITION 1	EXPERIMENT CONDITION 2	MATERIAL PROPERTIES1	MATERIAL PROPERTIES2
251	<chem>CCCC[Si](C)(OC)OC</chem>	0.407	20.6	2.09	19.8
⋮	⋮	⋮	⋮	⋮	⋮
CASE 3					
SERIAL No	STRUCTURAL FORMULA (SMILES)	EXPERIMENT CONDITION 1	EXPERIMENT CONDITION 2	MATERIAL PROPERTIES1	MATERIAL PROPERTIES2
670	<chem>CCO[Si](OCC)(OCC)N(CC)CC</chem>	1.06	56.4	5.18	-8.07
⋮	⋮	⋮	⋮	⋮	⋮

Fig. 5

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PLEASE DESIGNATE CHEMICAL SPACE.

☒ COMPOUND (CASE 1)	☒ COMPOUND (CASE 2)
☐ COMPOUND (CASE 3)	☐ COMPOUND (CASE 4)
☒ COMPOUND (CASE 5)	☒ COMPOUND (CASE 6)
☒ COMPOUND (CASE 7)	☐ COMPOUND (CASE 8)
☐ COMPOUND (CASE 9)	☒ COMPOUND (CASE 10)

OK

CANCEL

Fig. 6

CASE 2	
SERIAL No.	STRUCTURAL FORMULA (SMILES)
1	<chem>CO[Si](C)(OC)N1CCCCC1</chem>
2	<chem>CCN(CC)[Si](C)(OC)OC</chem>
3	<chem>O=C1C=CC(=O)C=C1</chem>
⋮	⋮
CASE 3	
SERIAL No.	STRUCTURAL FORMULA (SMILES)
251	<chem>CCCC[Si](C)(OC)OC</chem>
⋮	⋮
CASE 5	
SERIAL No.	STRUCTURAL FORMULA (SMILES)
670	<chem>CCO[Si](OCC)(OCC)N(CC)CC</chem>
⋮	⋮

Fig. 7

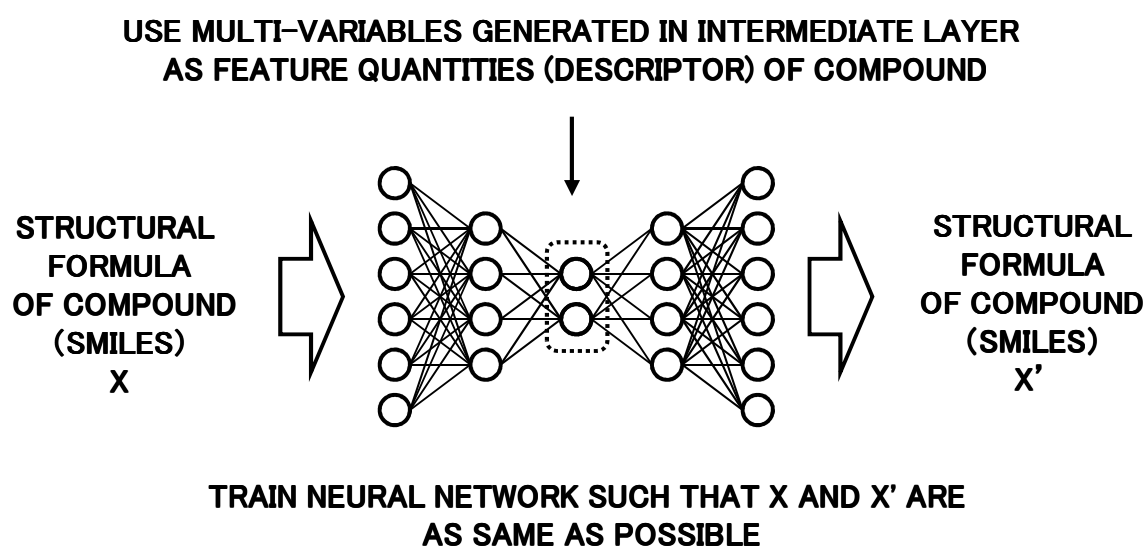


Fig. 8

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LIST OF MATERIALS TO BE SUBJECTED TO PROPERTY PREDICTION
HAS BEEN UPLOADED.

FILE:

BROWSE

OK

CANCEL

Fig. 9

No.	STRUCTURAL FORMULA (SMILES)
1	<chem>CO[Si](C)(OC)N1CCCCC1</chem>
2	<chem>CCN(CC)[Si](C)(OC)OC</chem>
3	<chem>O=C1C=CC(=O)C=C1</chem>
⋮	⋮

Fig. 10

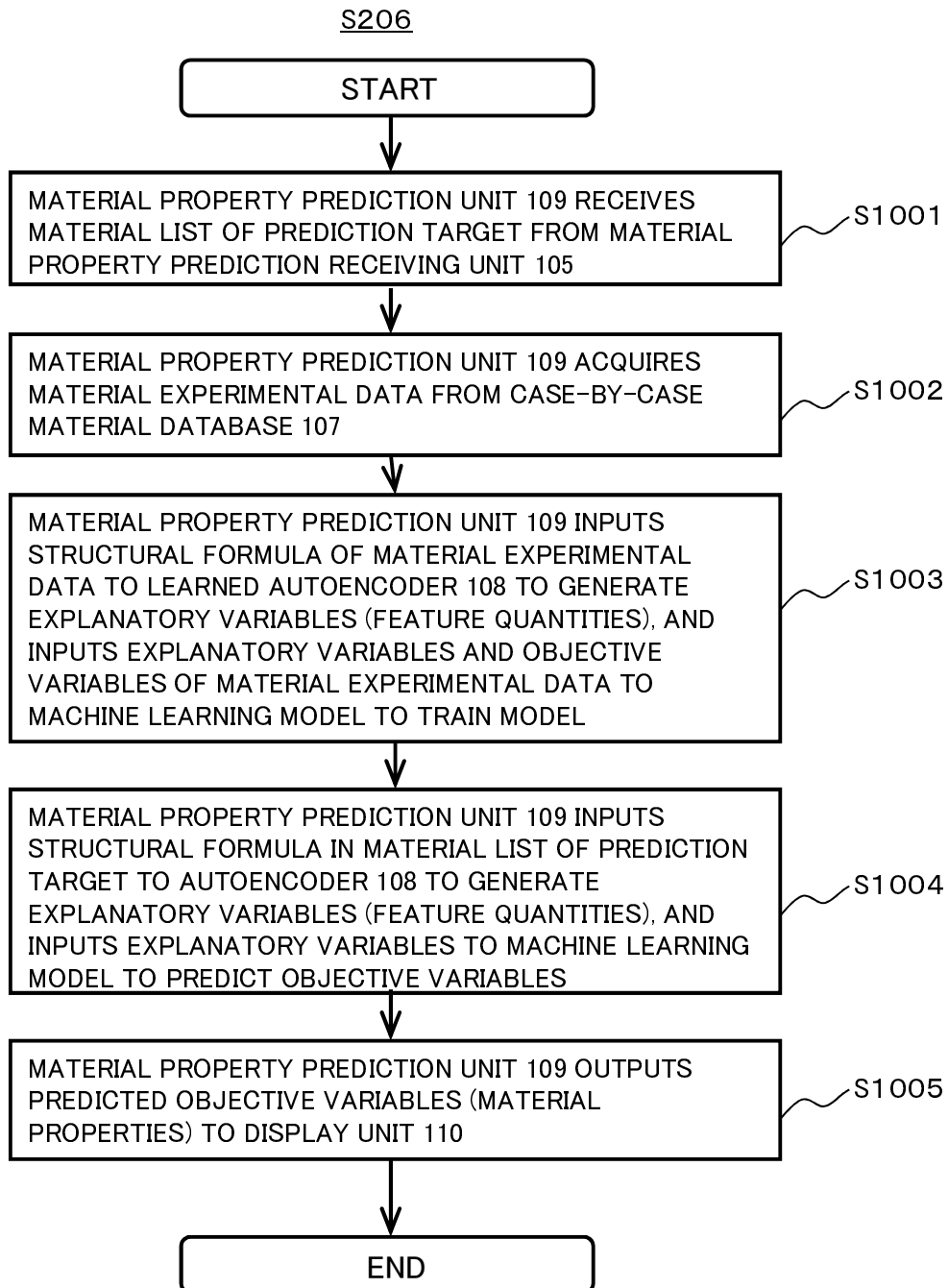


Fig. 11

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MATERIAL PROPERTY PREDICTION RESULT

No.	STRUCTURAL FORMULA (SMILES)	MATERIAL PROPERTIES 1	MATERIAL PROPERTIES 2
1	<chem>CO[Si](C)(OC)N1CCCCC1</chem>	4.12	-12.5
2	<chem>CCN(CC)[Si](C)(OC)OC</chem>	1.56	29.1
3	<chem>O=C1C=CC(=O)C=C1</chem>	-0.374	35.5
⋮	⋮	⋮	⋮

STORAGE

END

Fig. 12

