

DFT design of new materials

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GB1302743.8, US 2014/177578, EP14153898.3

GB1307533.8, US 2014/223465, EP14161255.6

GB1307535.3

US 2013/0052077 A1

Acta Materialia 61, 3378 (2013)

Intermetallics 48, 62 (2014)

Theory of Condensed Matter Group, Department of Physics

Routes to materials design

Experimental
databases:
accurate



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graph LR; A[Experimental databases: accurate] --> B(( )); C[Computational: all compositions] --> B; B --> D[Materials discovery];
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Computational:
all compositions

Materials
discovery

Routes to materials design

Experimental
databases:
accurate

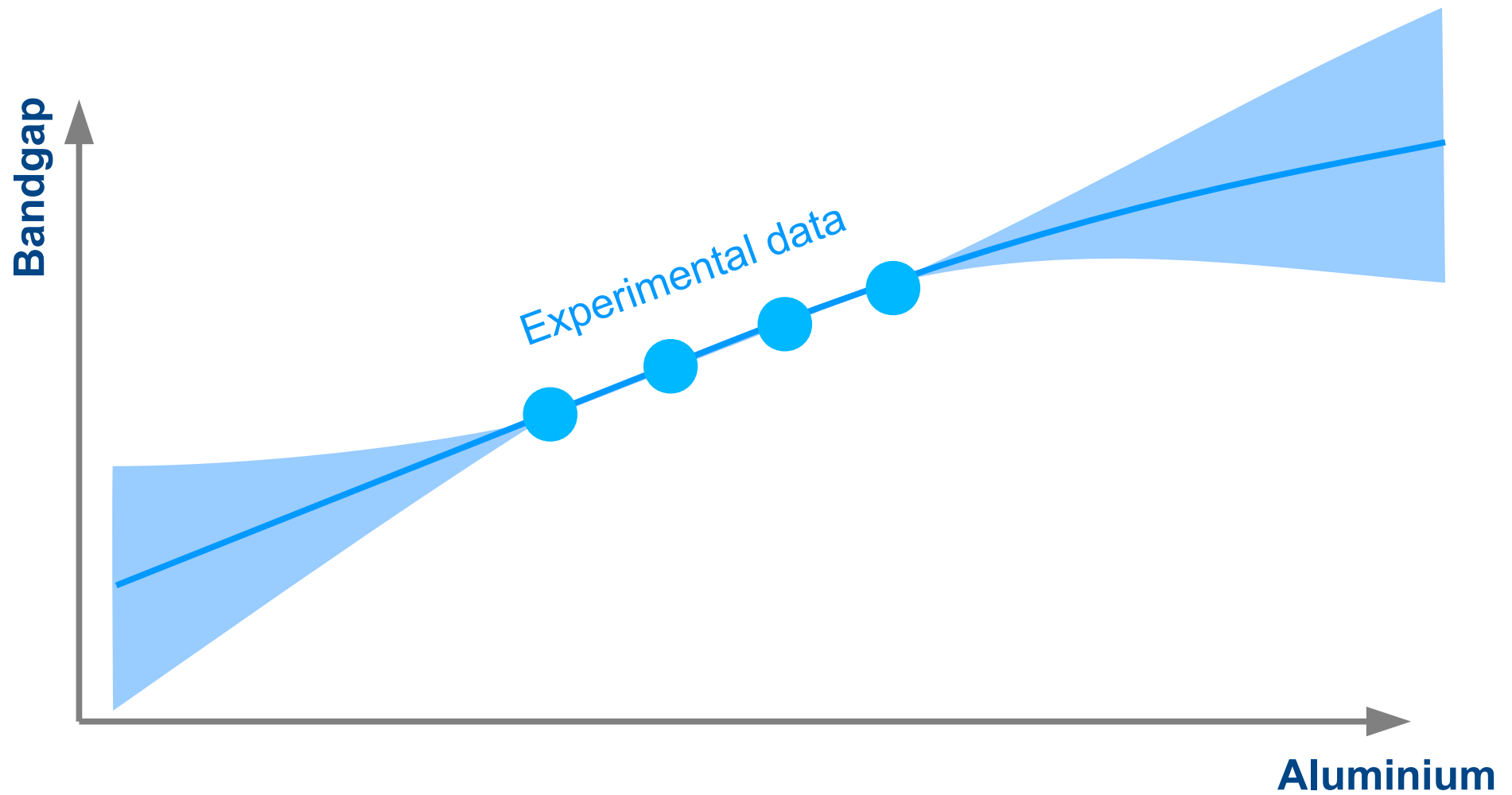
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graph LR; A[Experimental databases: accurate] --> B[Property correlations]; C[Computational: all compositions] --> B; B --> D[Materials discovery]
```

Property
correlations

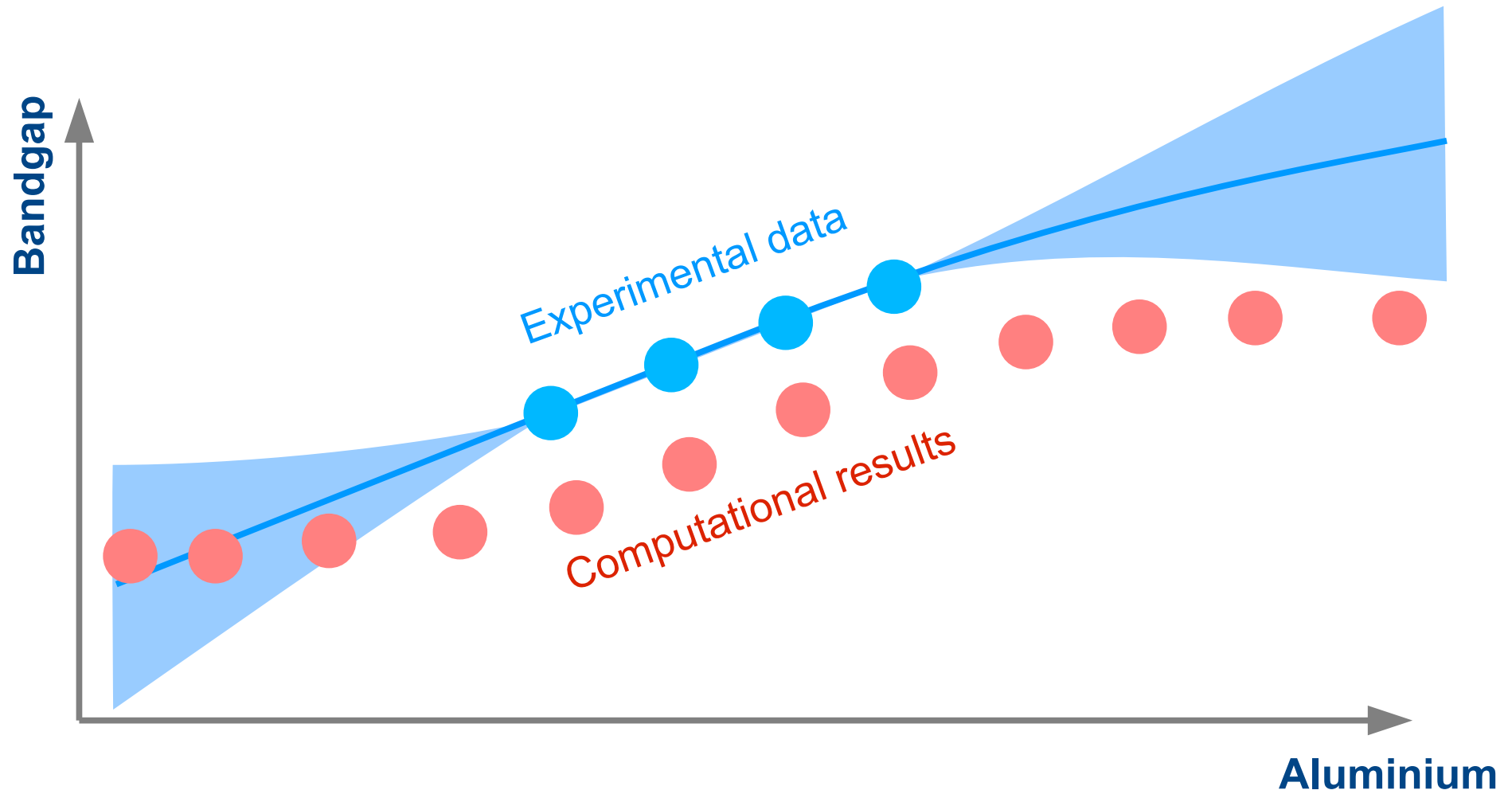
Materials
discovery

Computational:
all compositions

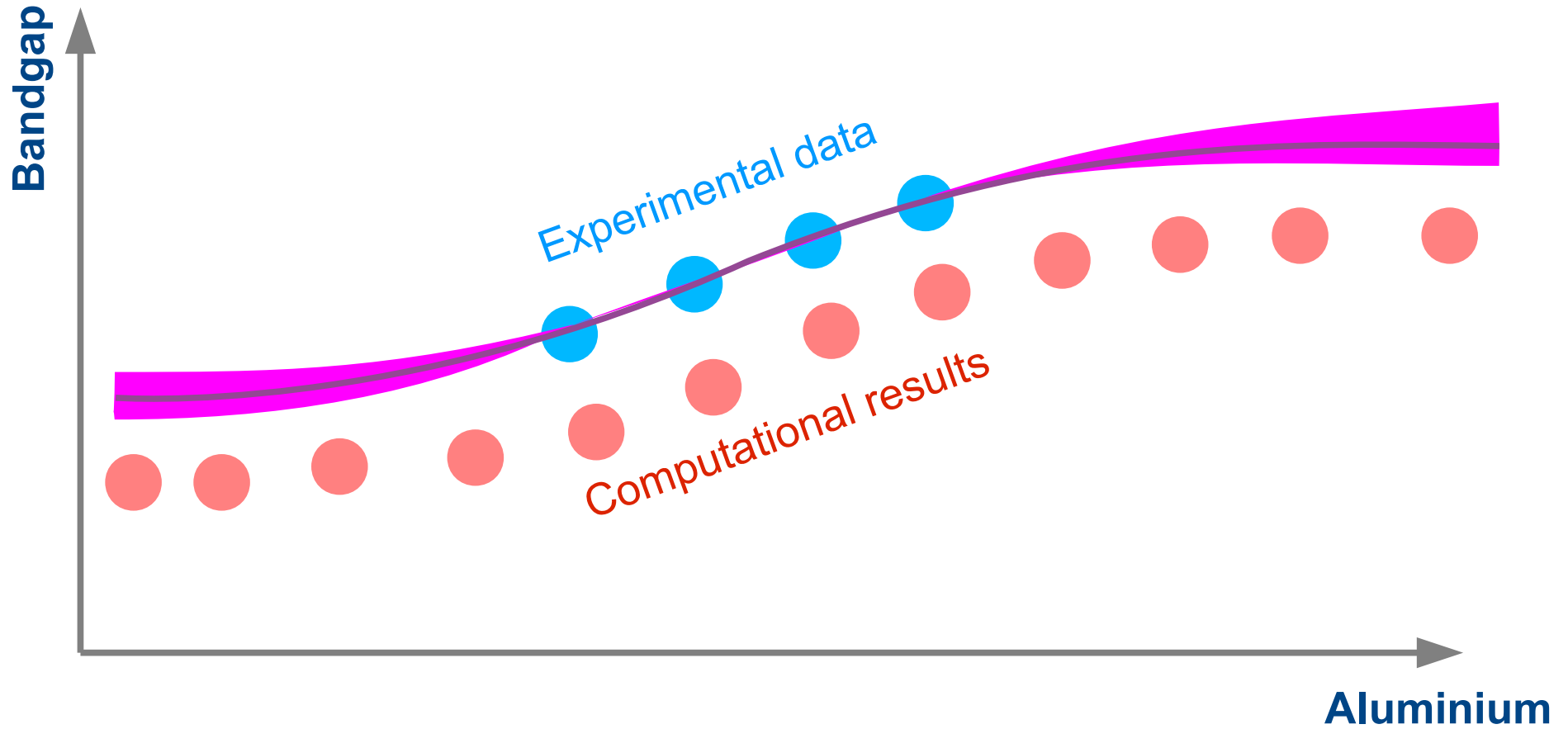
Exploiting correlations



Exploiting correlations



Exploiting correlations



Summary

Experimental databases: materials genome project

First principles calculations: DFT & proprietary Samsung tools

Exploit correlations to enable concurrent materials design