Is Band better than ADF?

The core of the issue

Introduction

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- What is Band?

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- Atomic sub shells
- Numerical atomic orbitals
- Properties
  - Energy
  - A tensor / finite nucleus
  - Density at nucleus

Band: 1D, 2D, 3D

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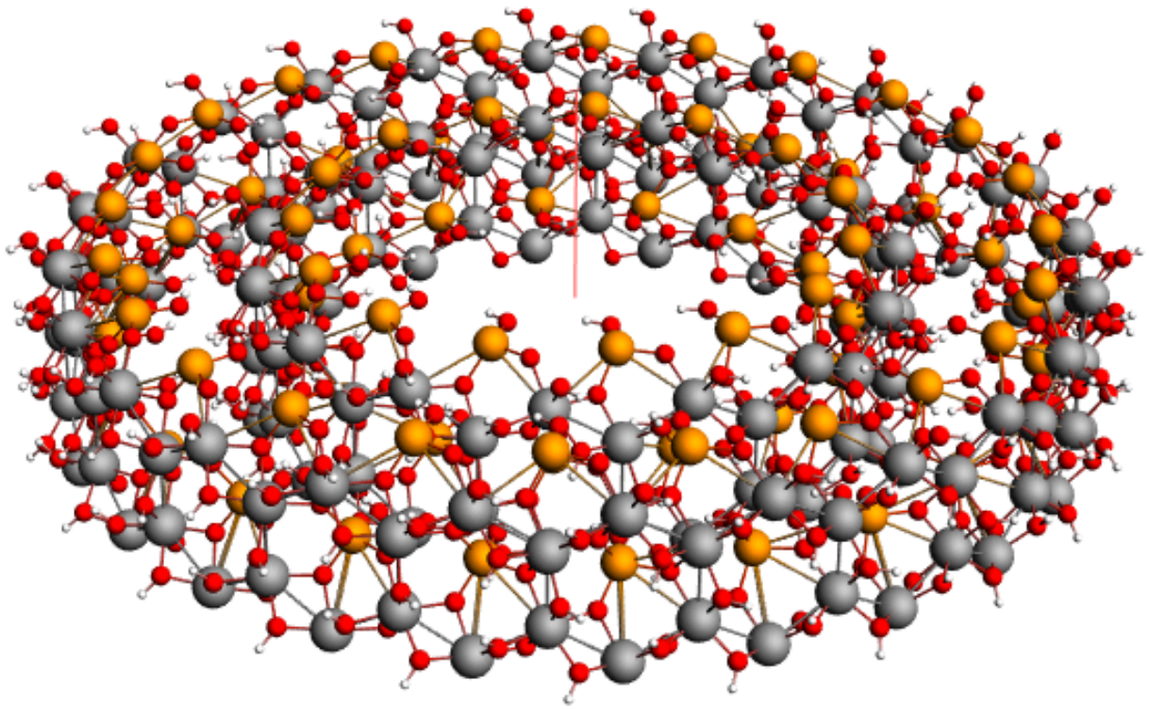
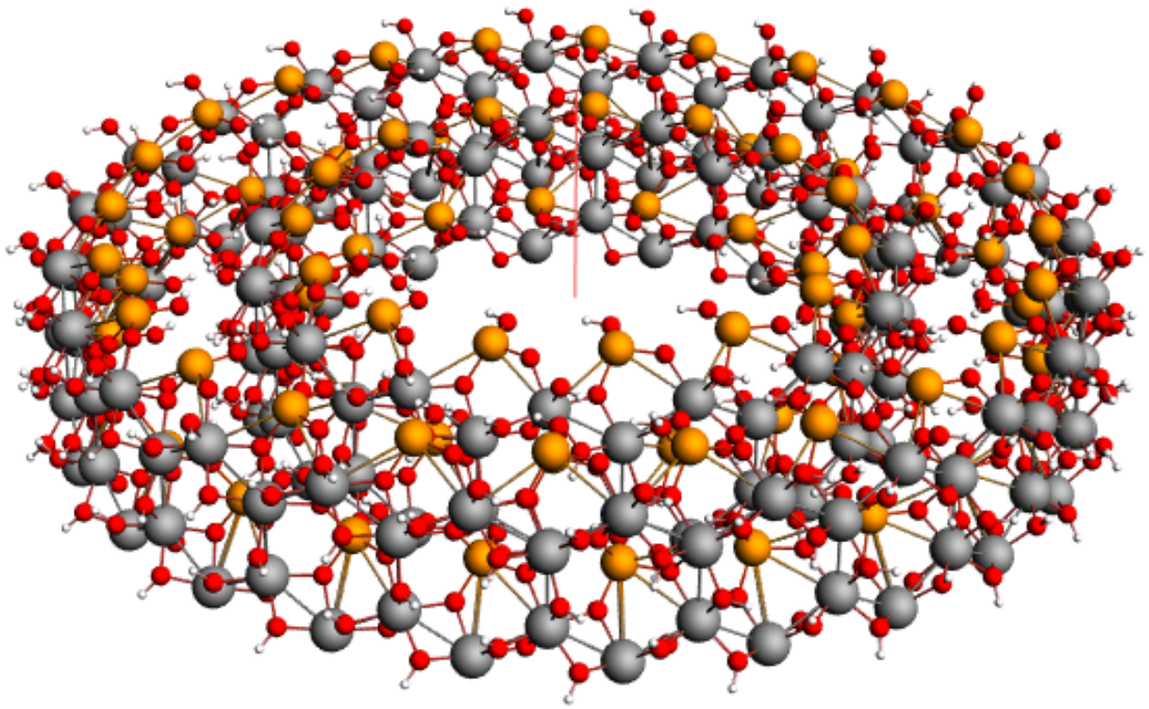


1D: double wall imogolite tube

Band: 1D, 2D, 3D



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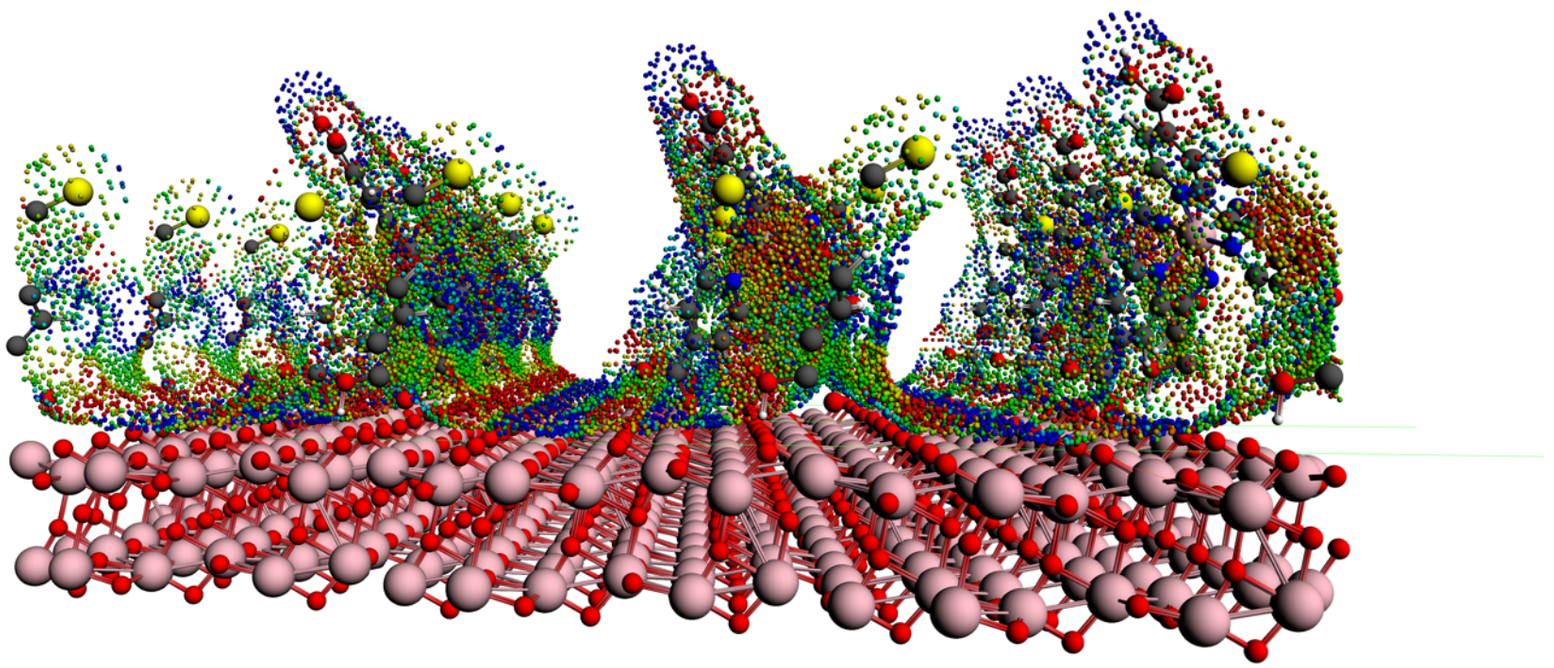
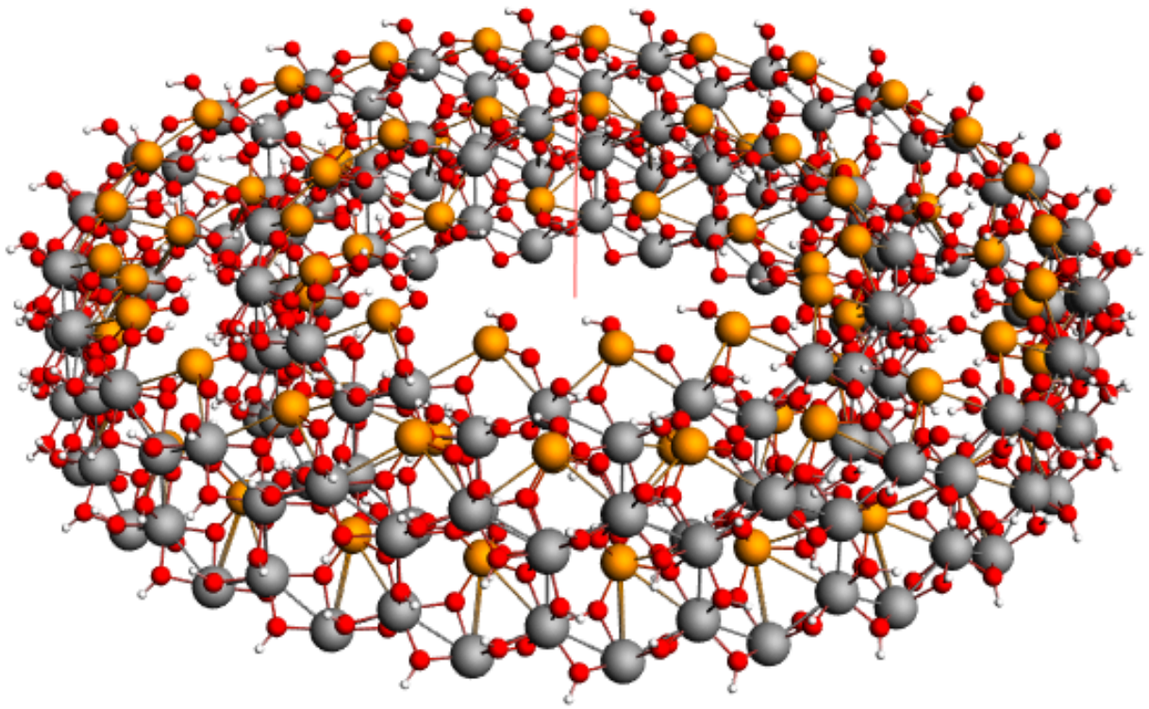


2D: Dye in solution on TiO2

Band: 1D, 2D, 3D



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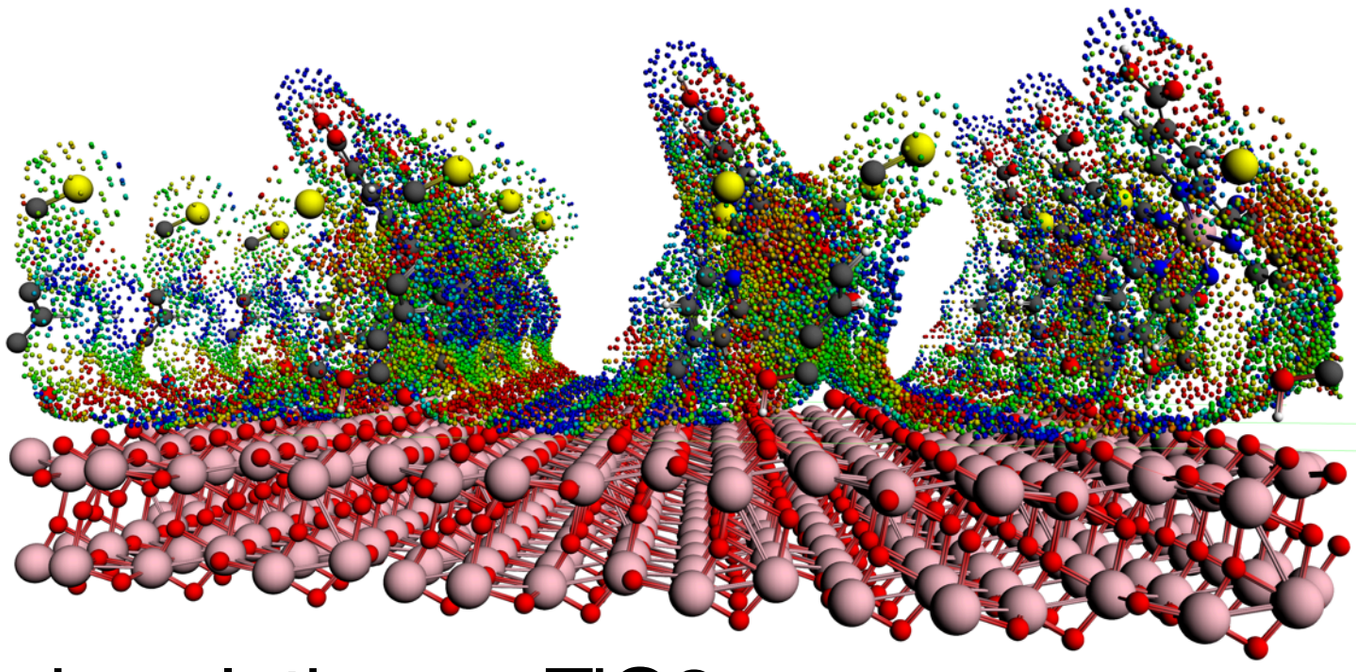

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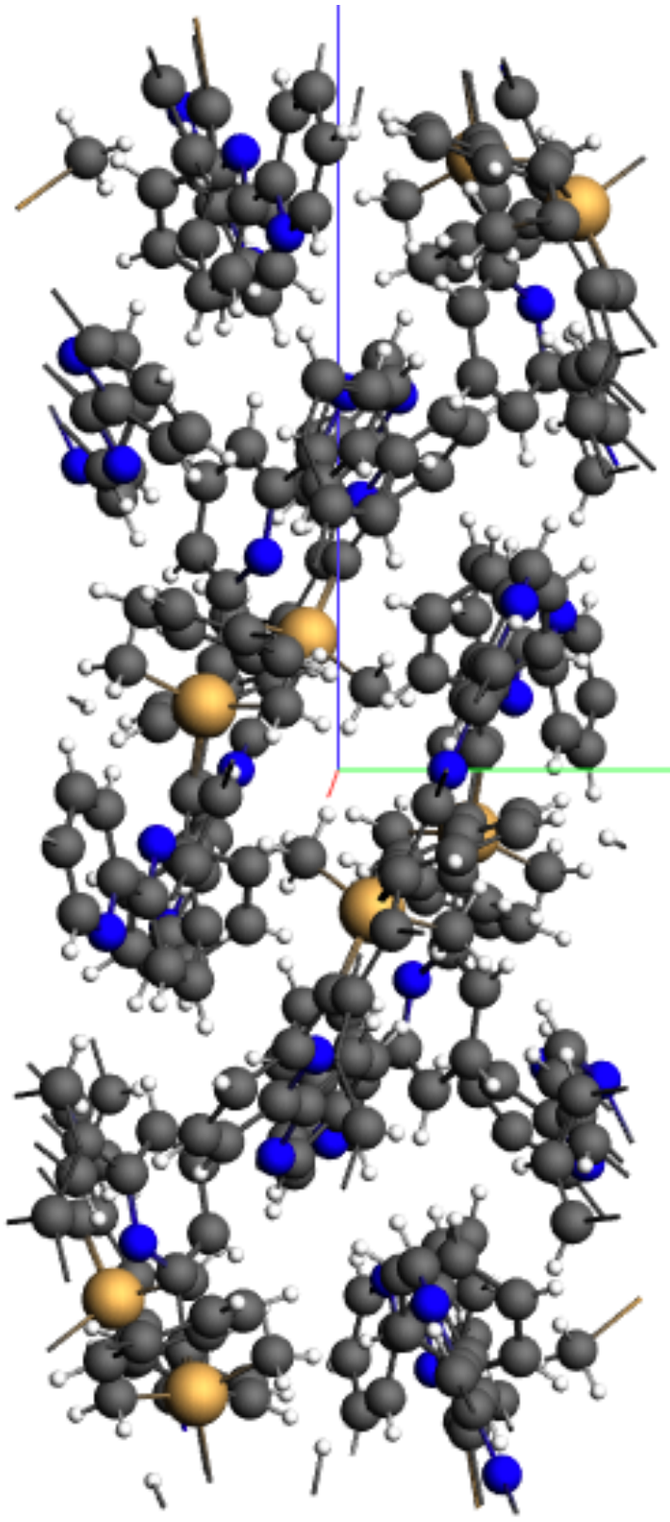

3D:OLED material

Key difference

	ADF	Band
Basis	STO	STO+NAO

Atomic Sub Shells

	Sub Shells (n,l)
H-He	1s
Li-Be	1s,2s
B-Ne	1s,2s,2p
Na-Mg	[Ne],3s
Al-Ar	[Ne],3s,3p
K-Ca	[Ar],4s
Sc-Zn	[Ar],4s,3d

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- User: SZ<DZ<TZP<TZ2P<QZ4P

Numerical Basis

$$\chi_{nlm} = R_{nl}(r) \;\; Y_{lm}(\Omega)$$

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- Radial part is STO or NAO
- NAO: solution of spherical atom on grid: `dirac` subroutine
- Very good approximation for core functions (and valence core wiggles?)

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- QZ: replace STO with most overlap

In short

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- Band: Mixture of NAO and STOs

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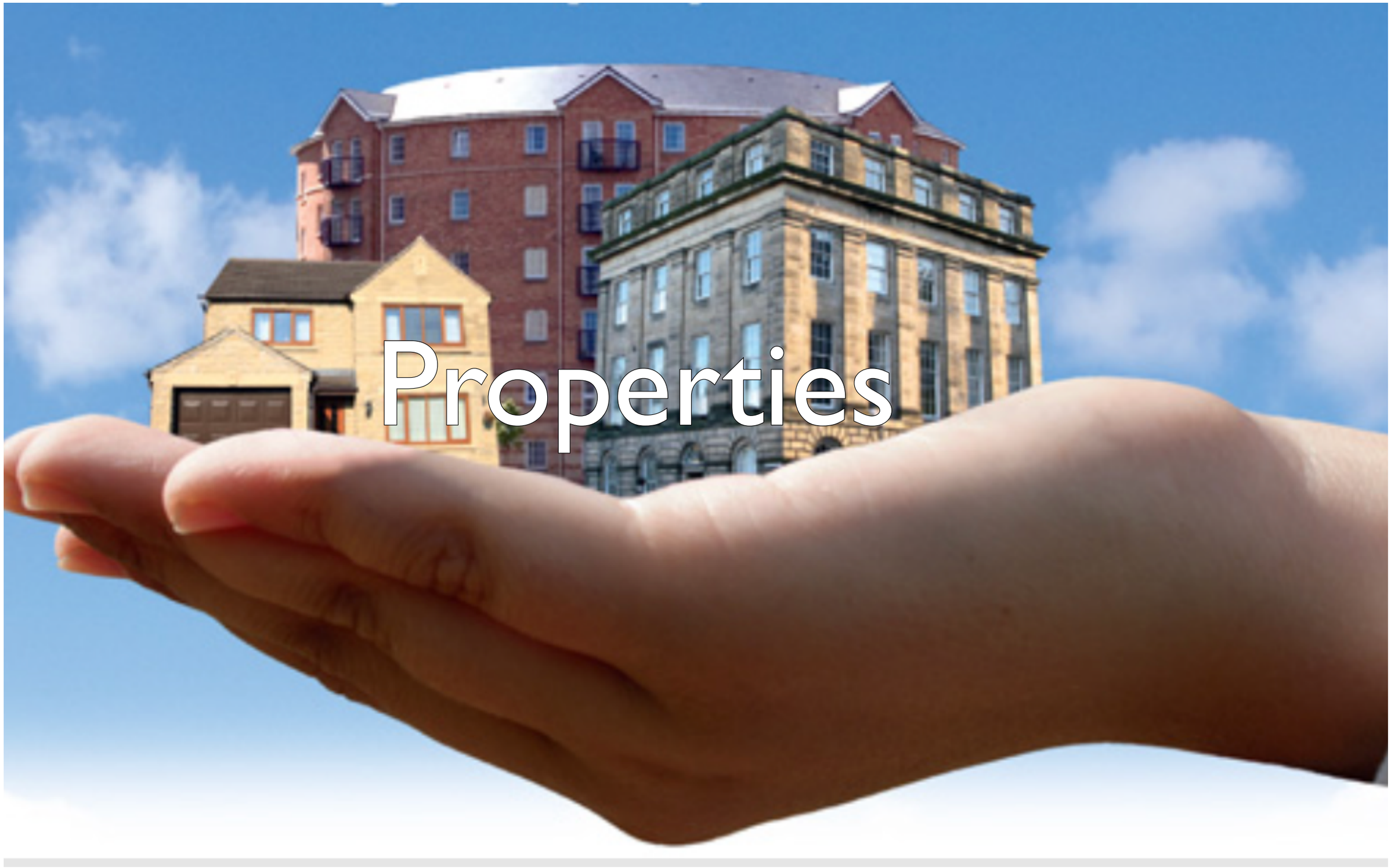
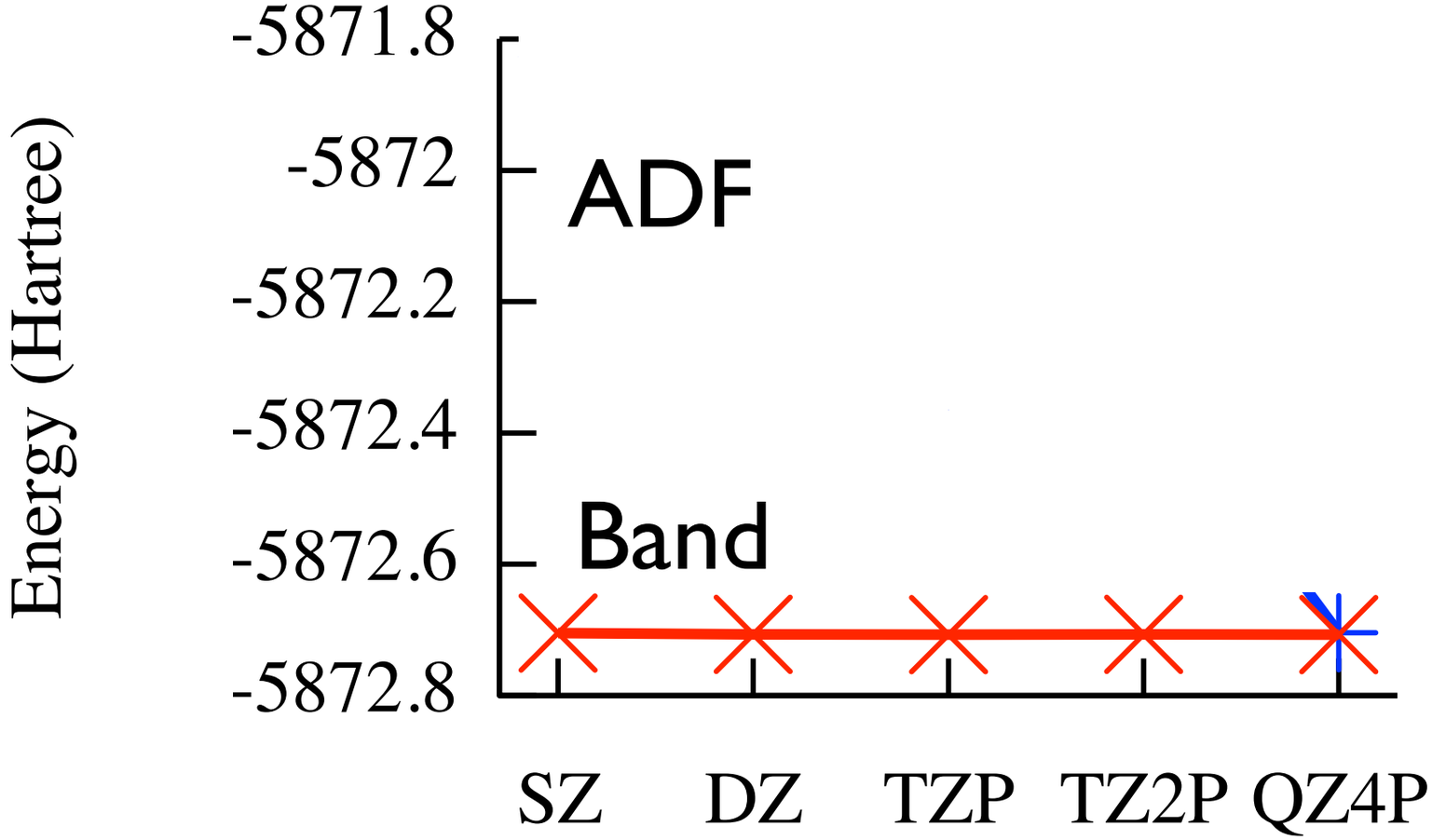
- ADF: STO functions
- Band: Mixture of NAO and STOs
- Which one performs better?


Properties

Total Energy...

Rb_2 molecule



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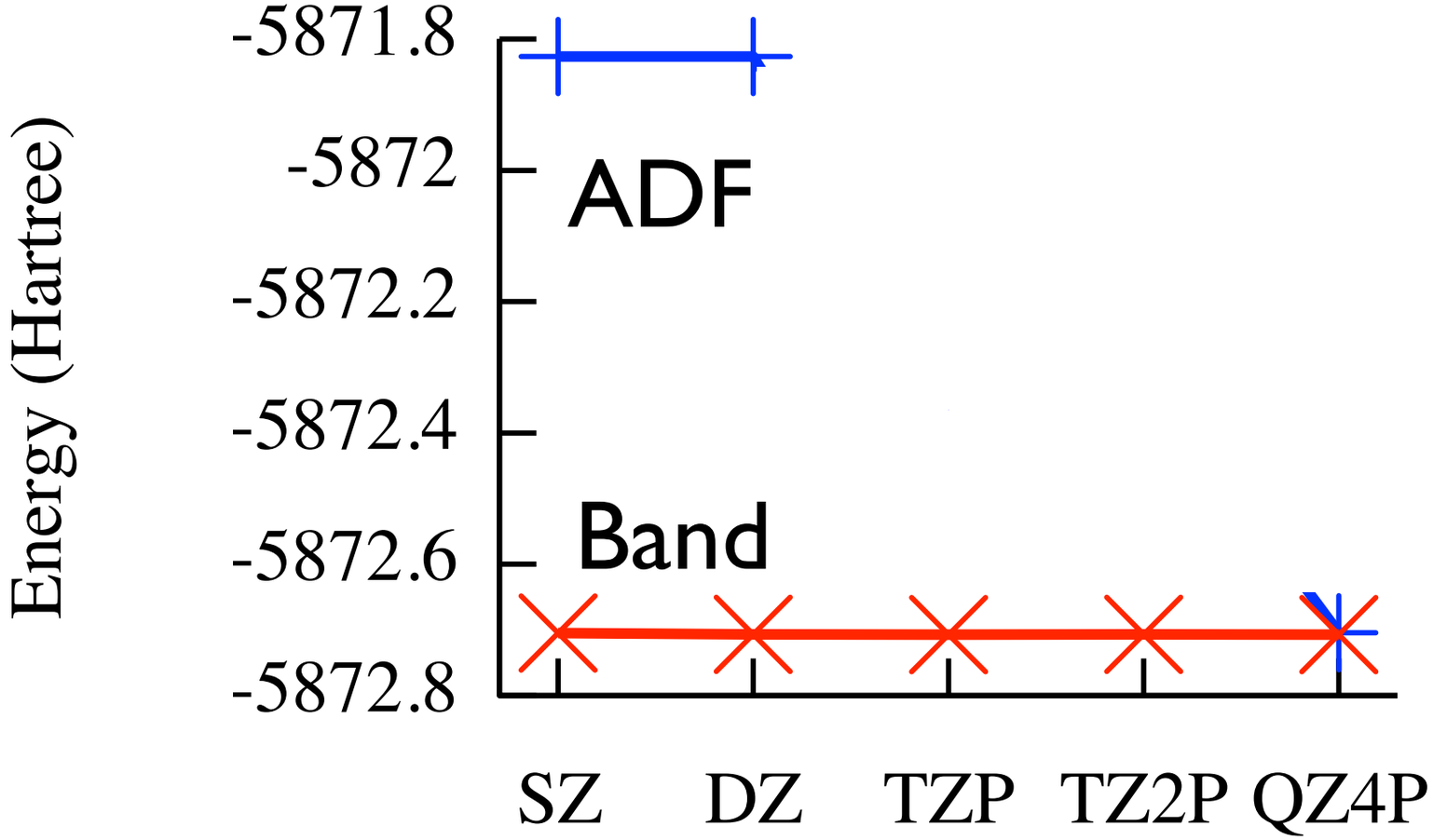

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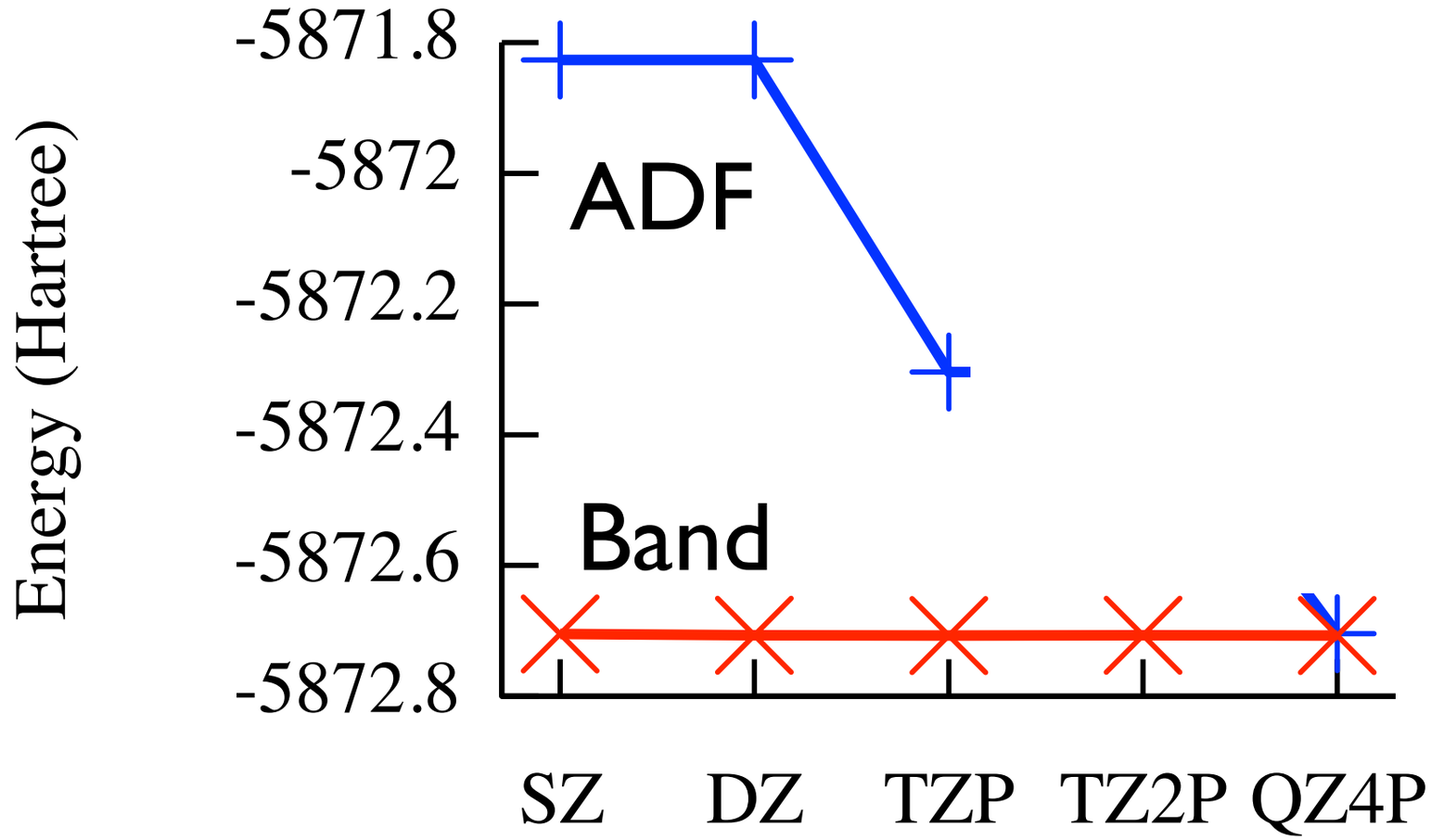

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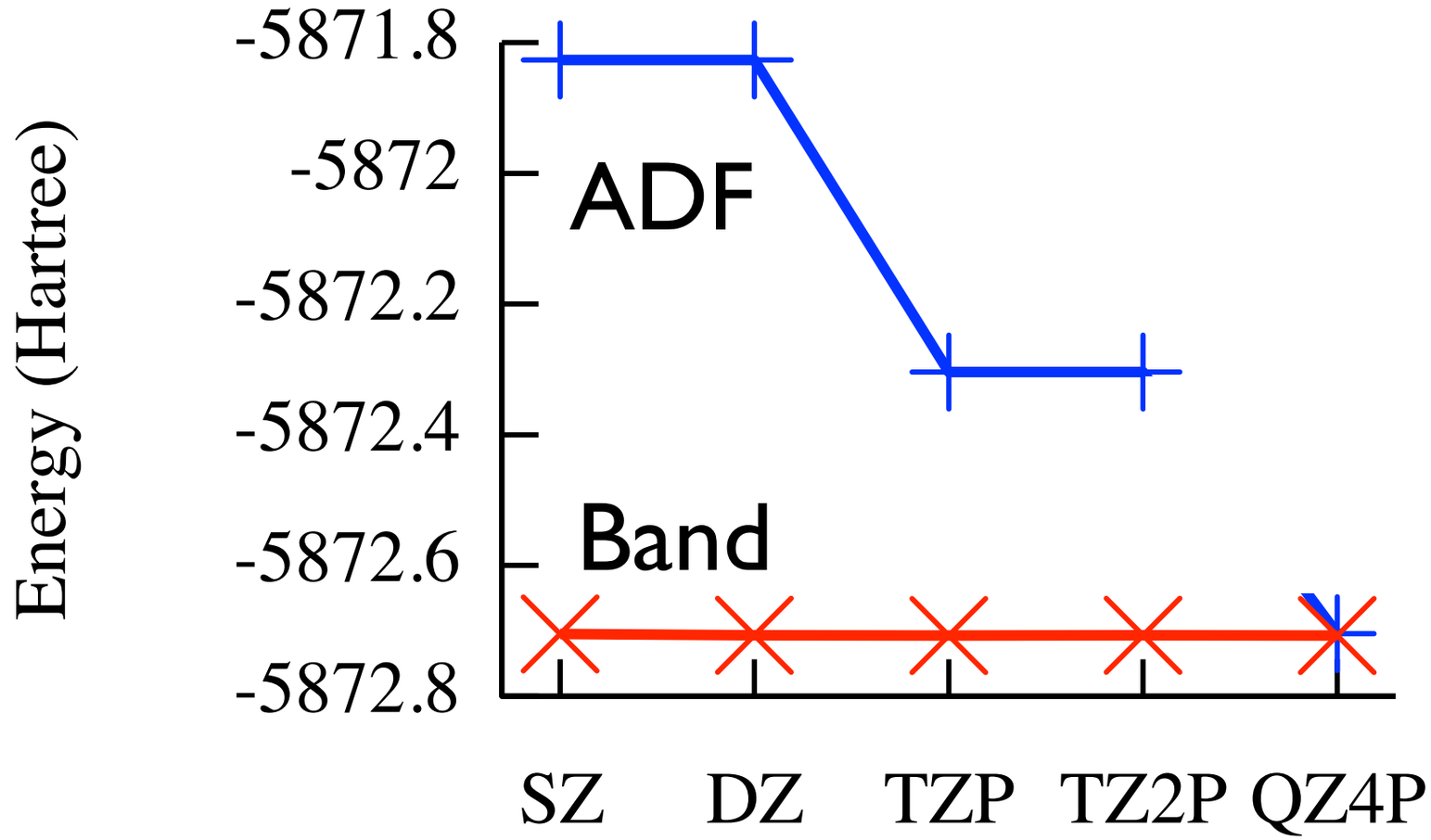

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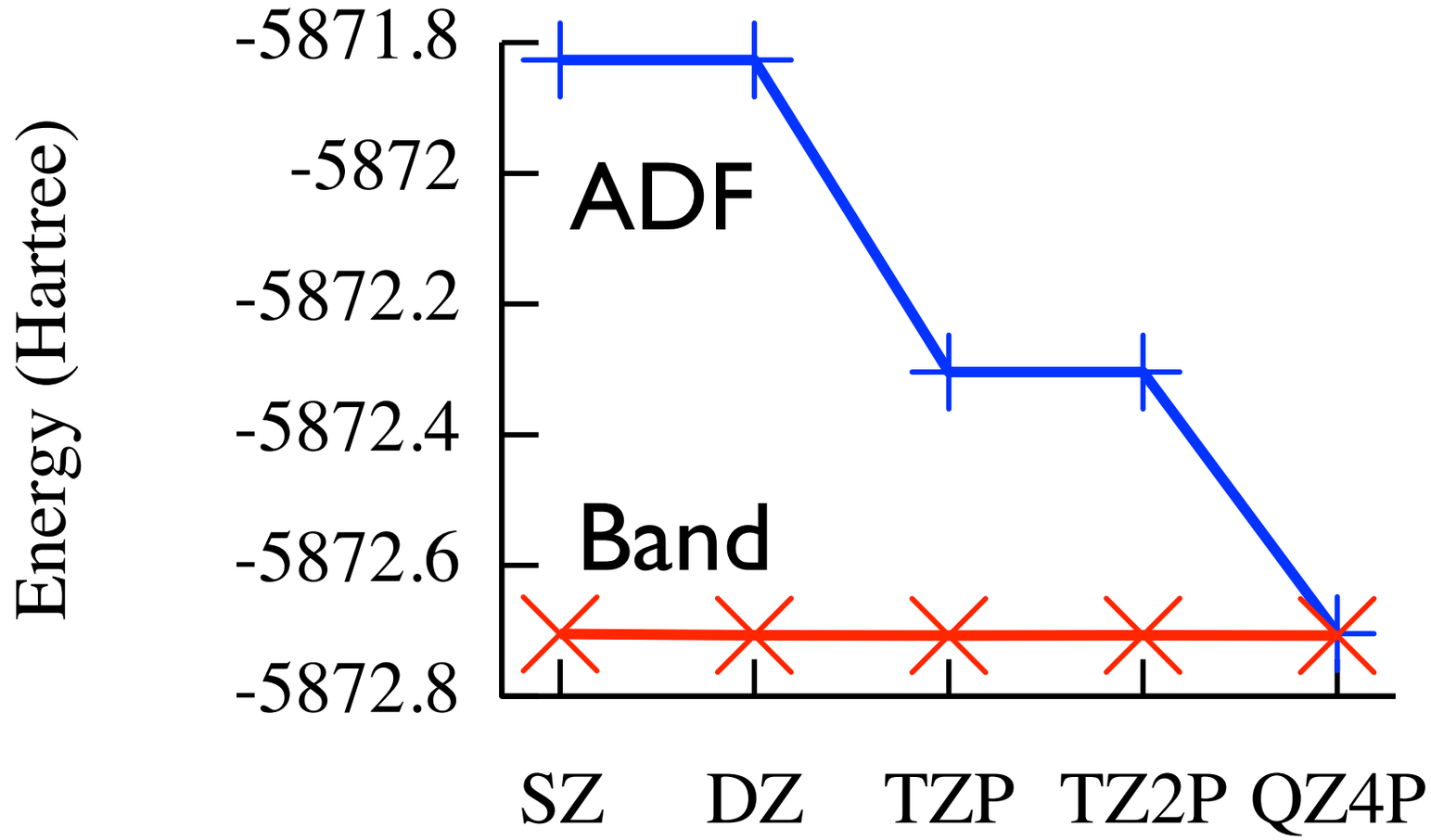

...Bond Energy

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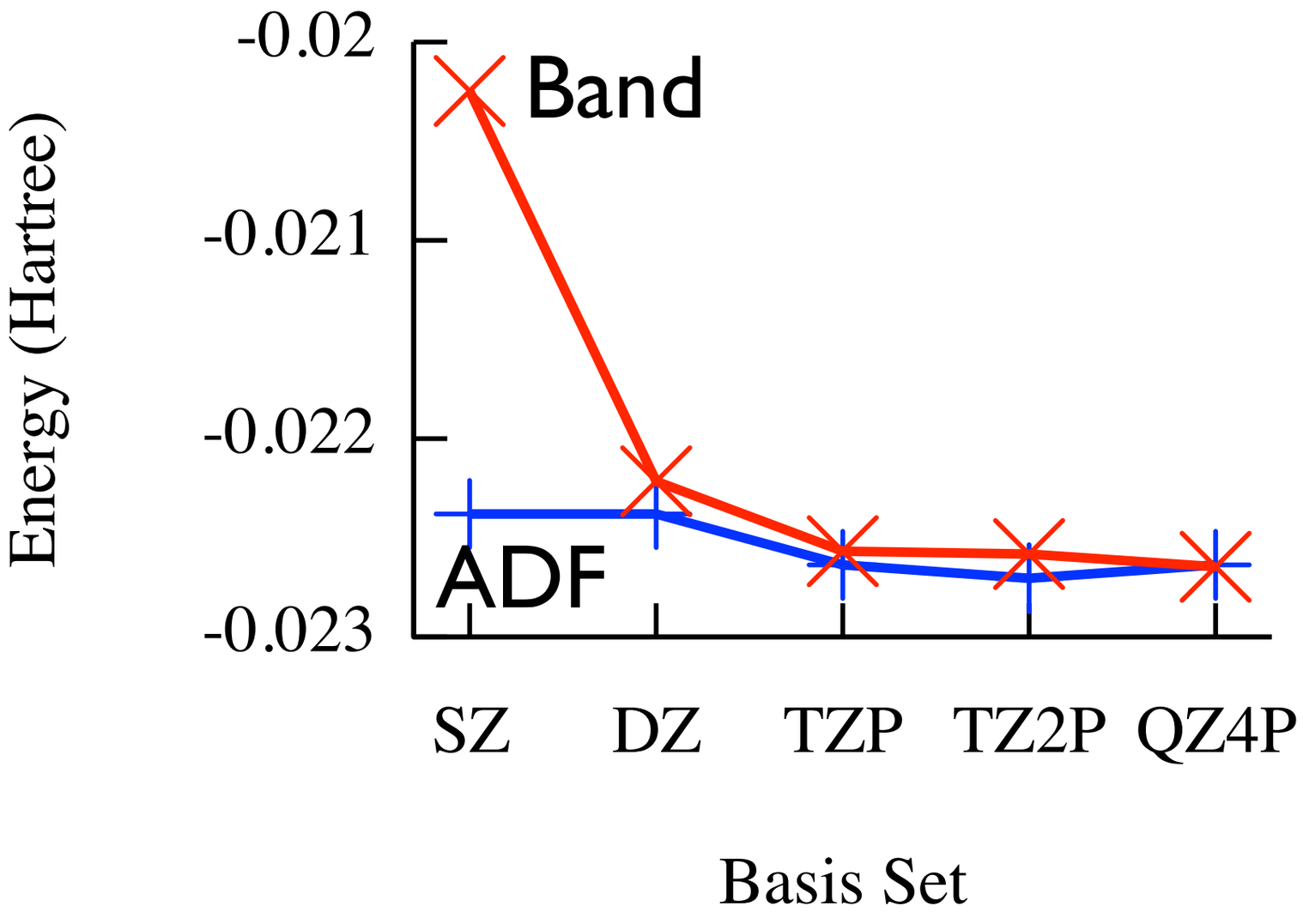
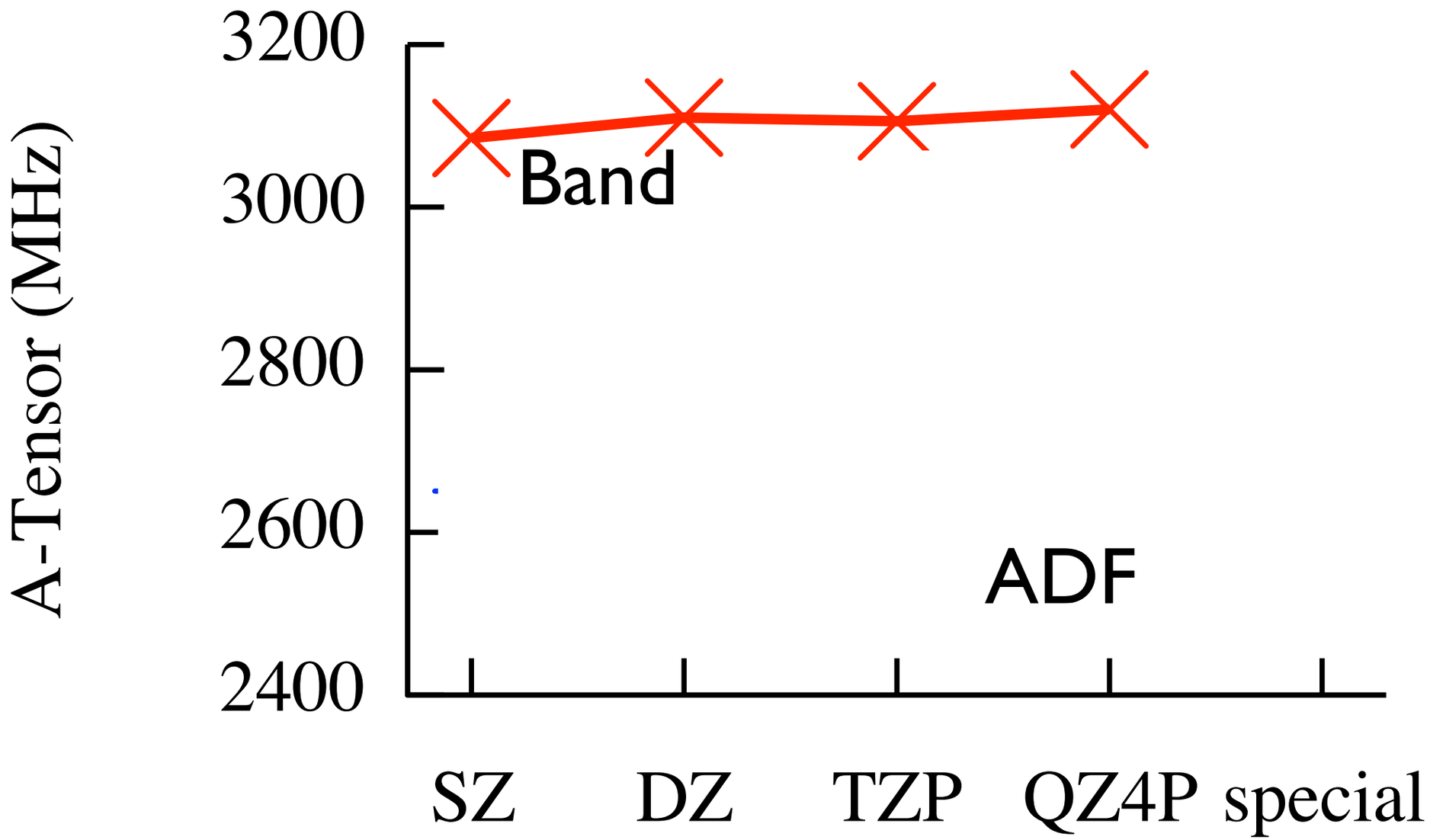


A-tensor Au atom



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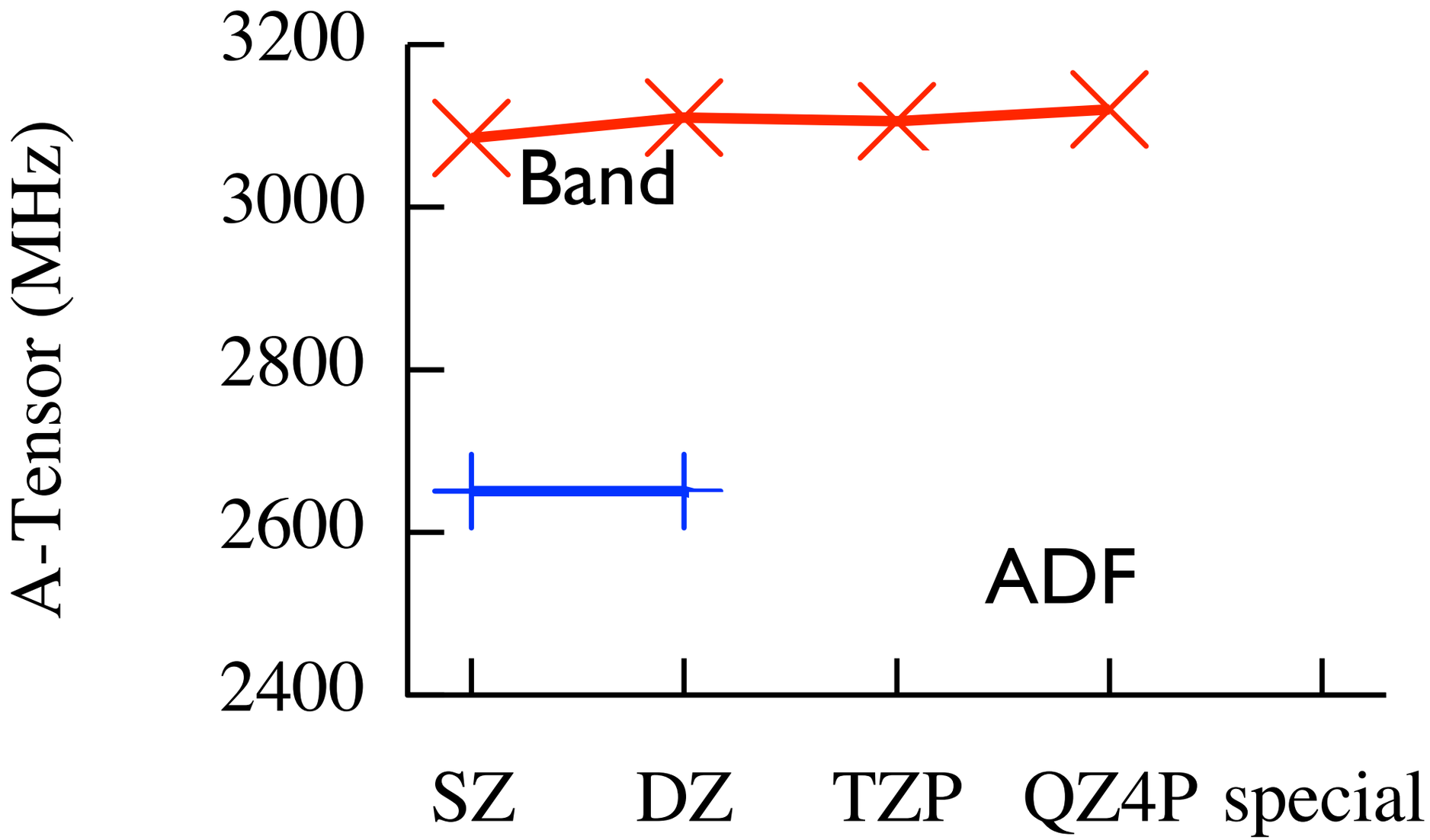

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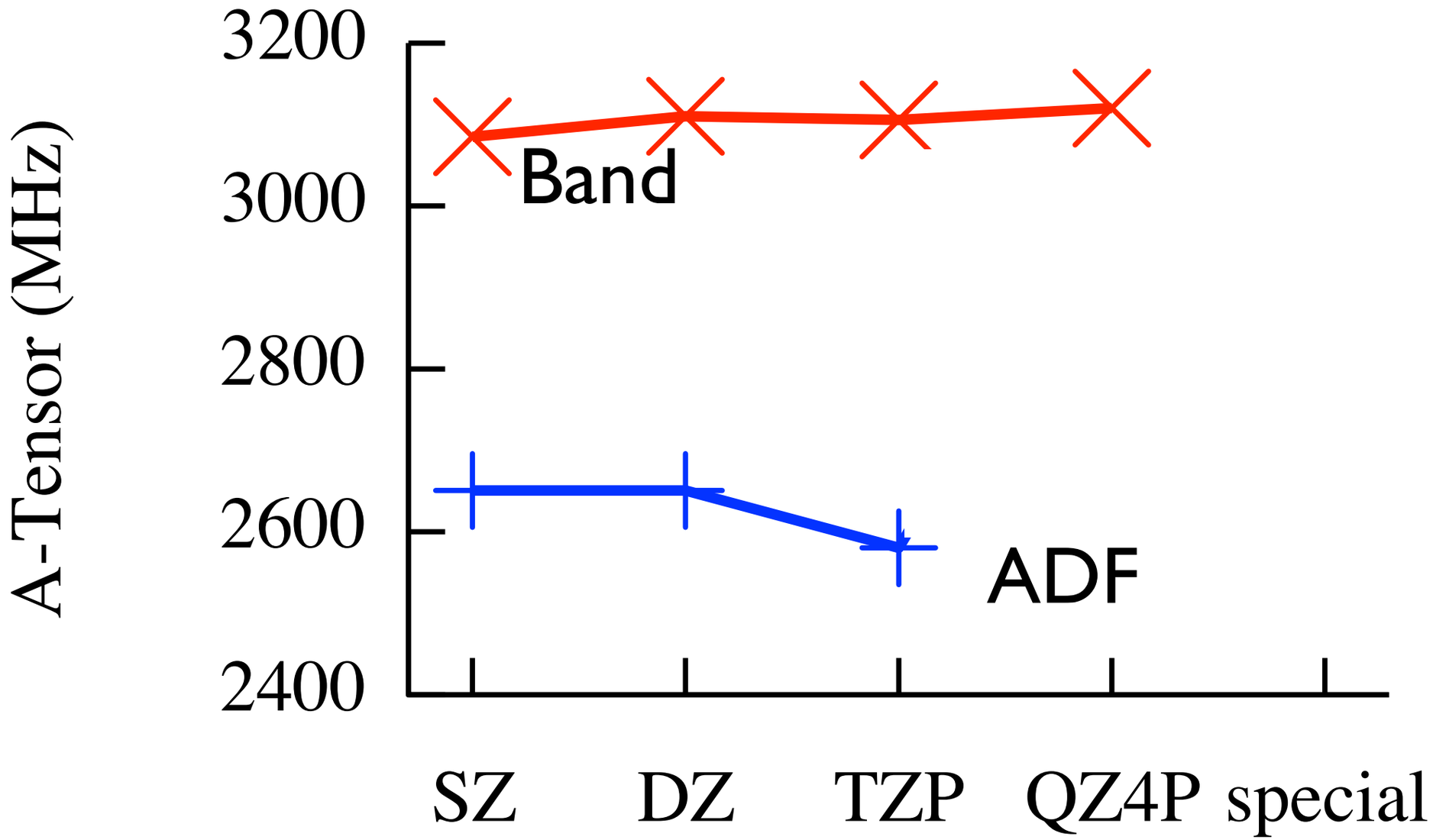

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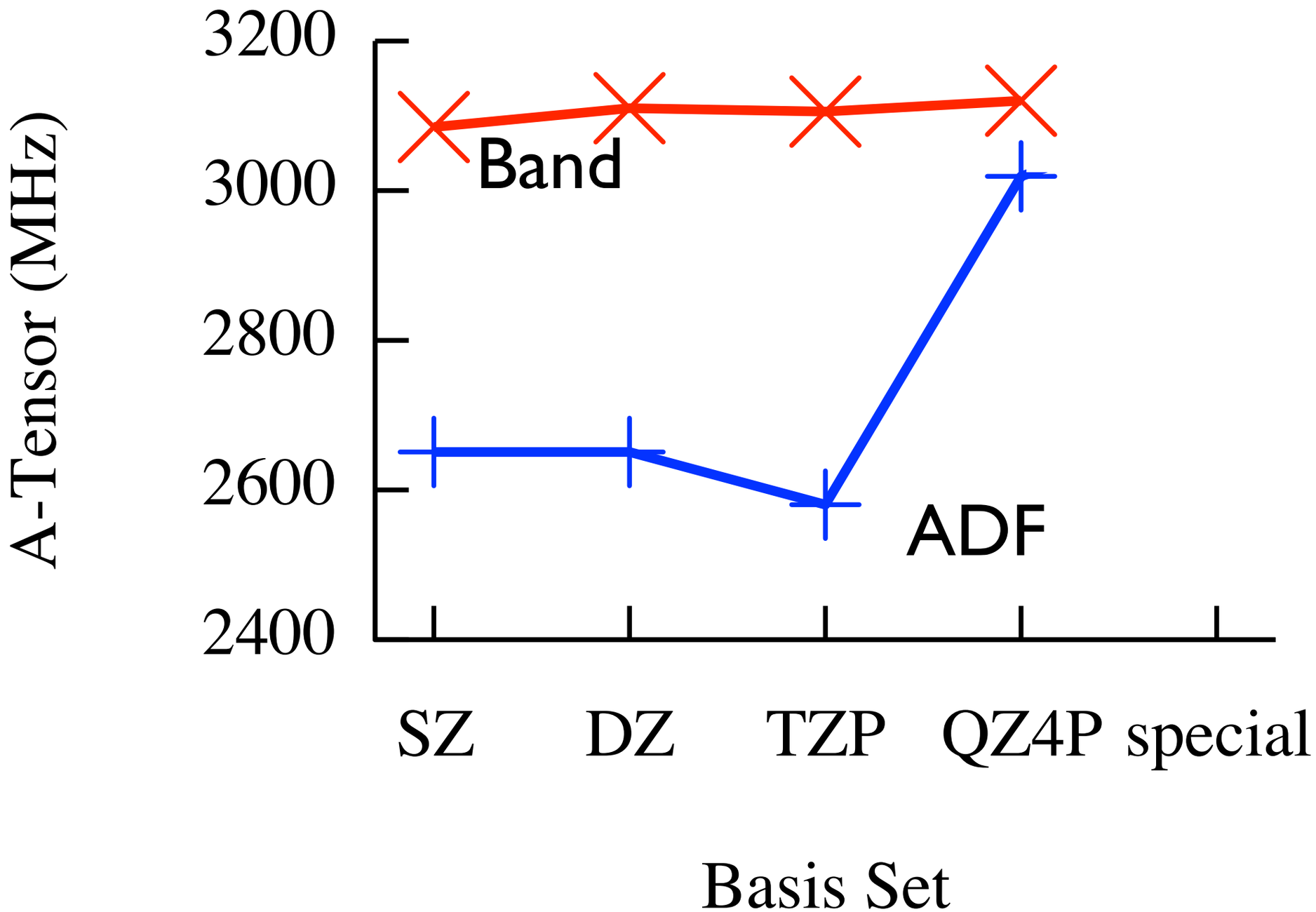

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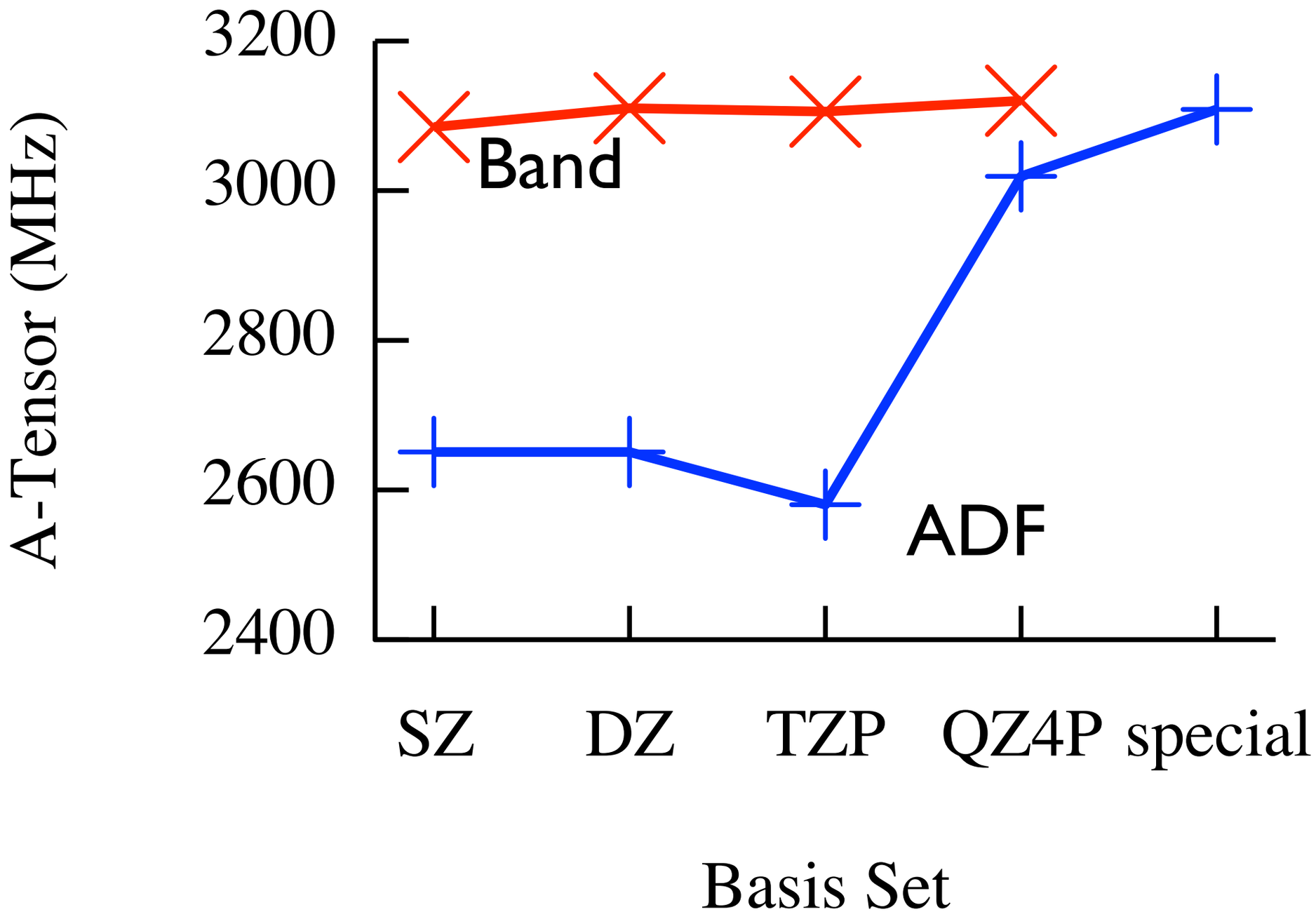

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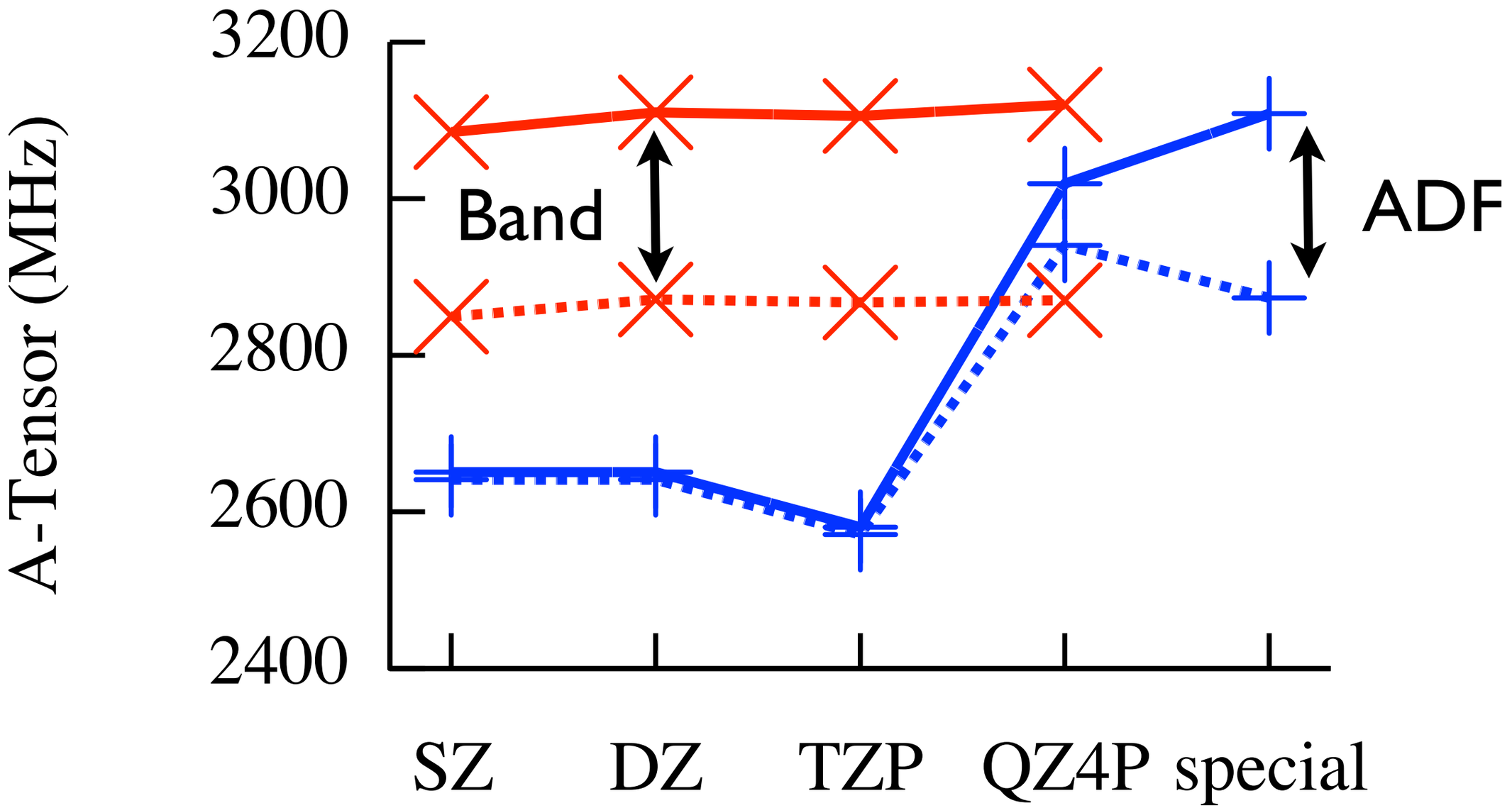
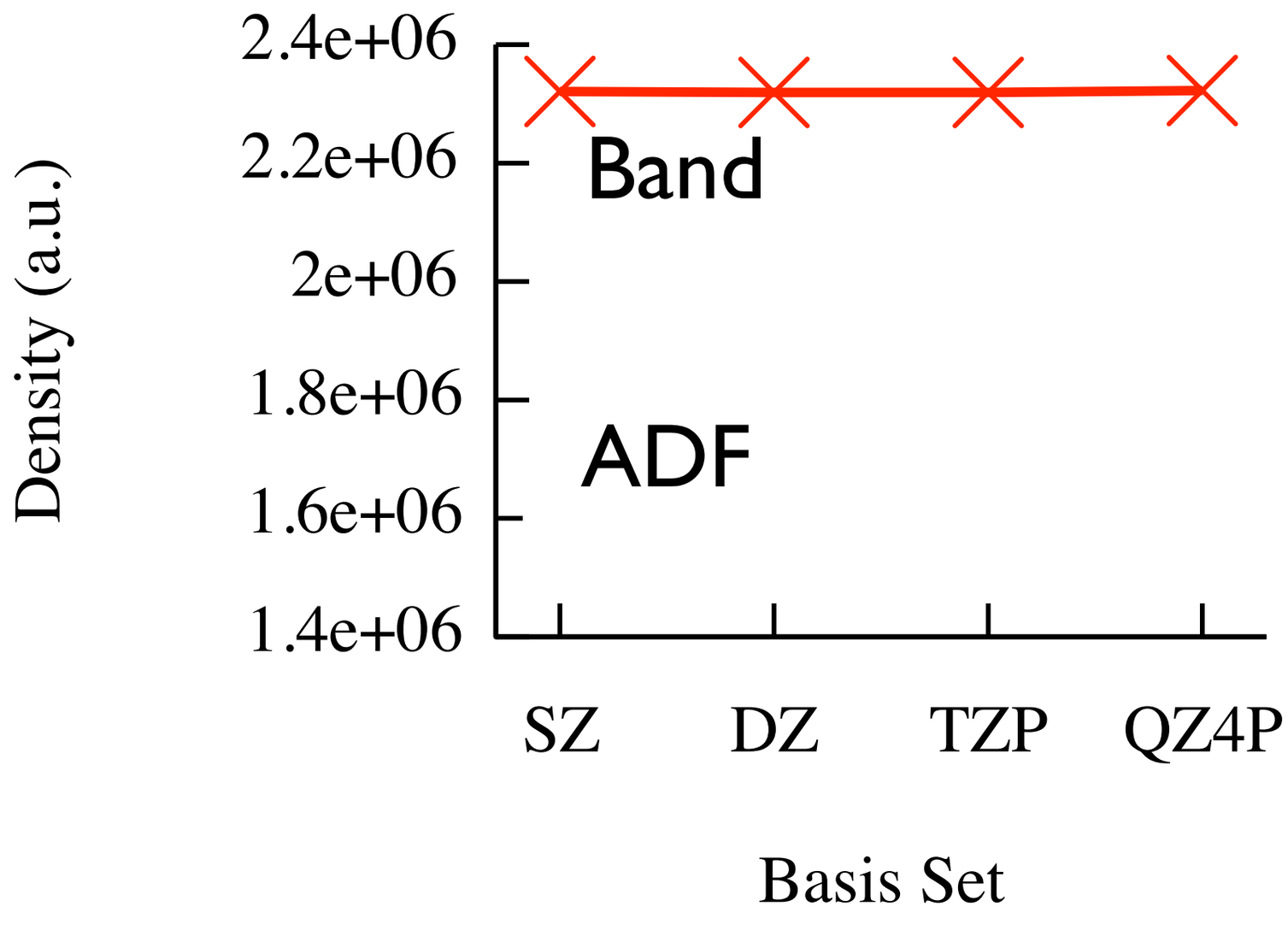
- Implemented: gaussian and homogeneous

Finite nucleus effect Au



Density at Nucleus

Au_2 molecule



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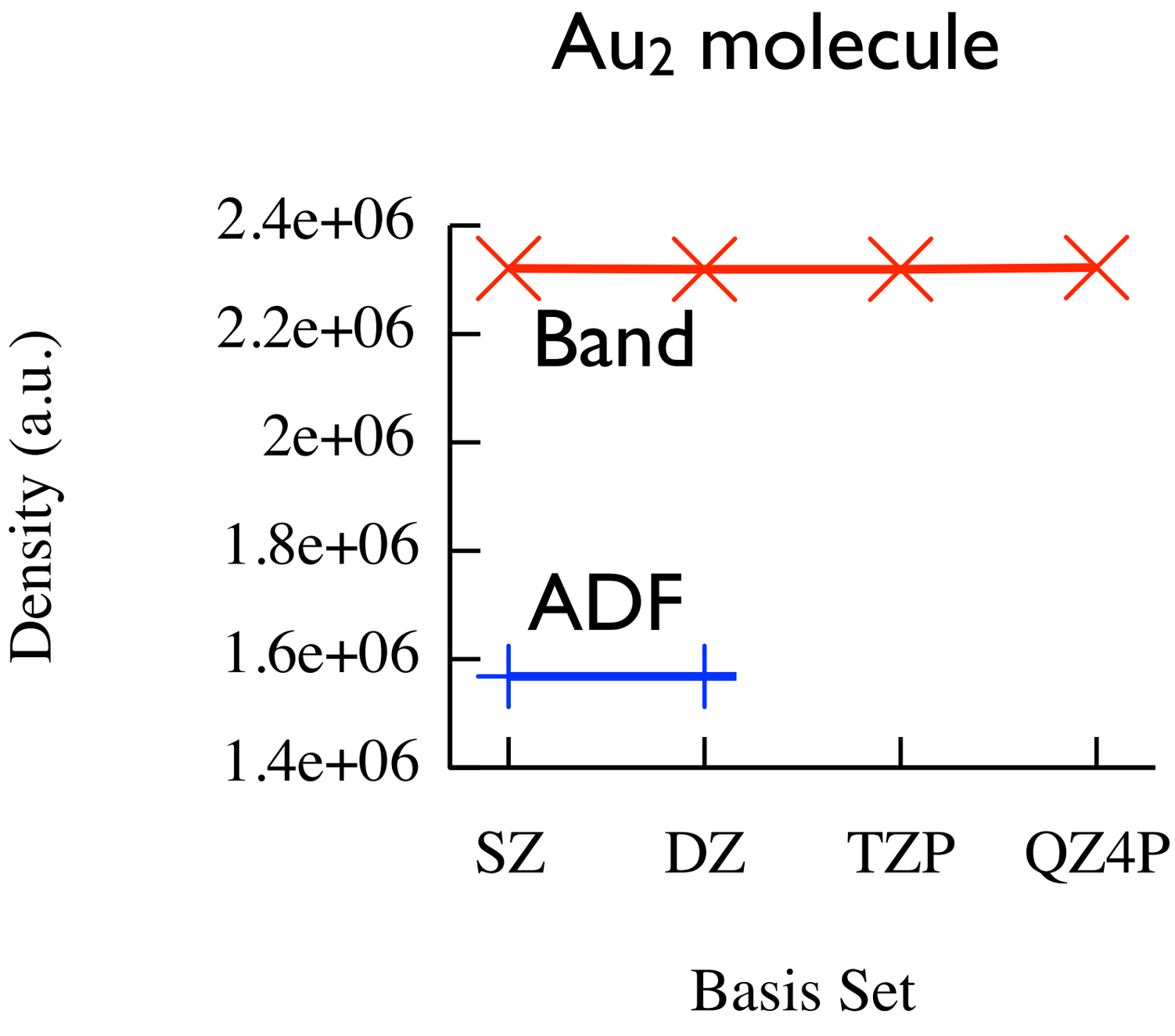

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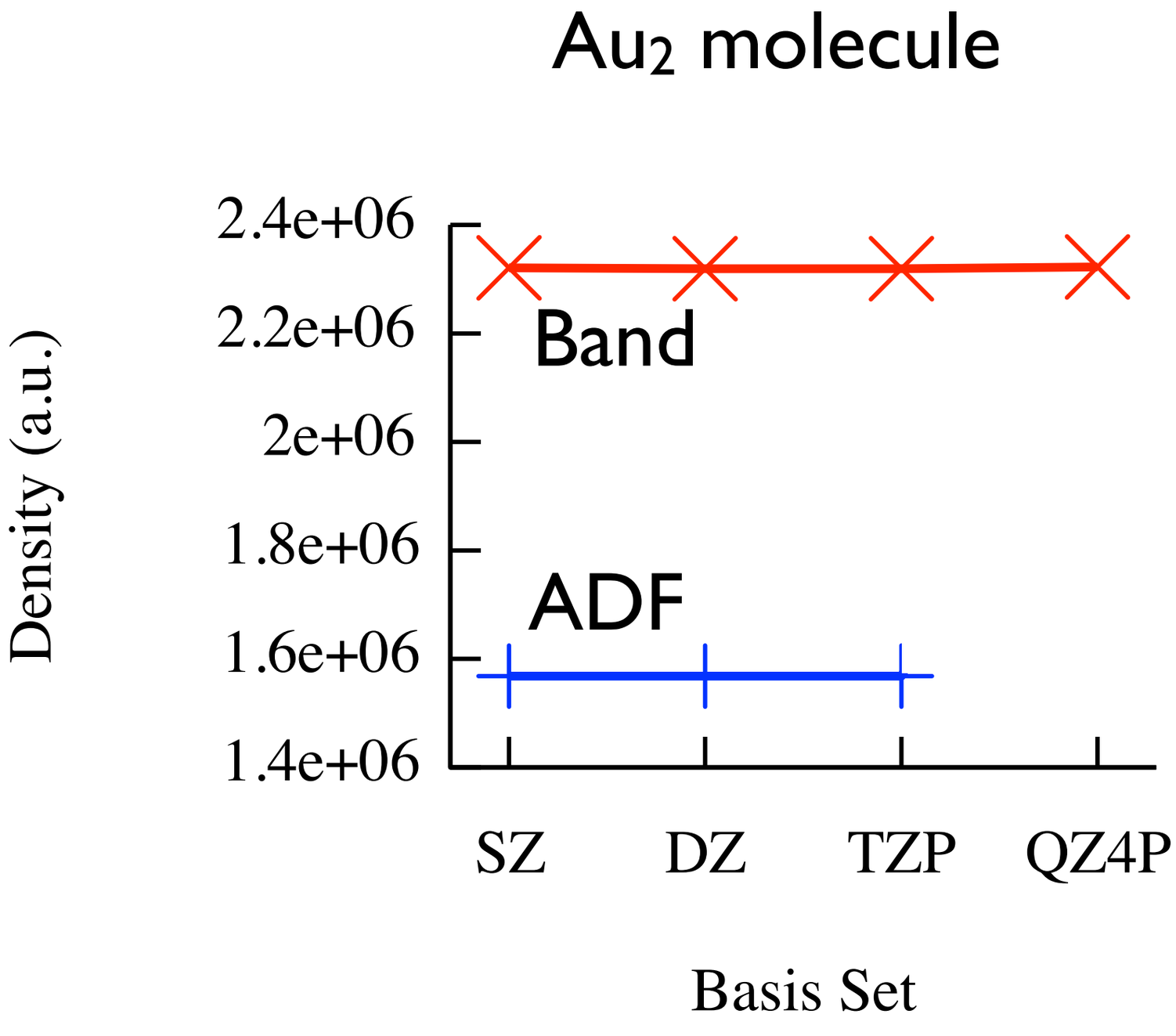

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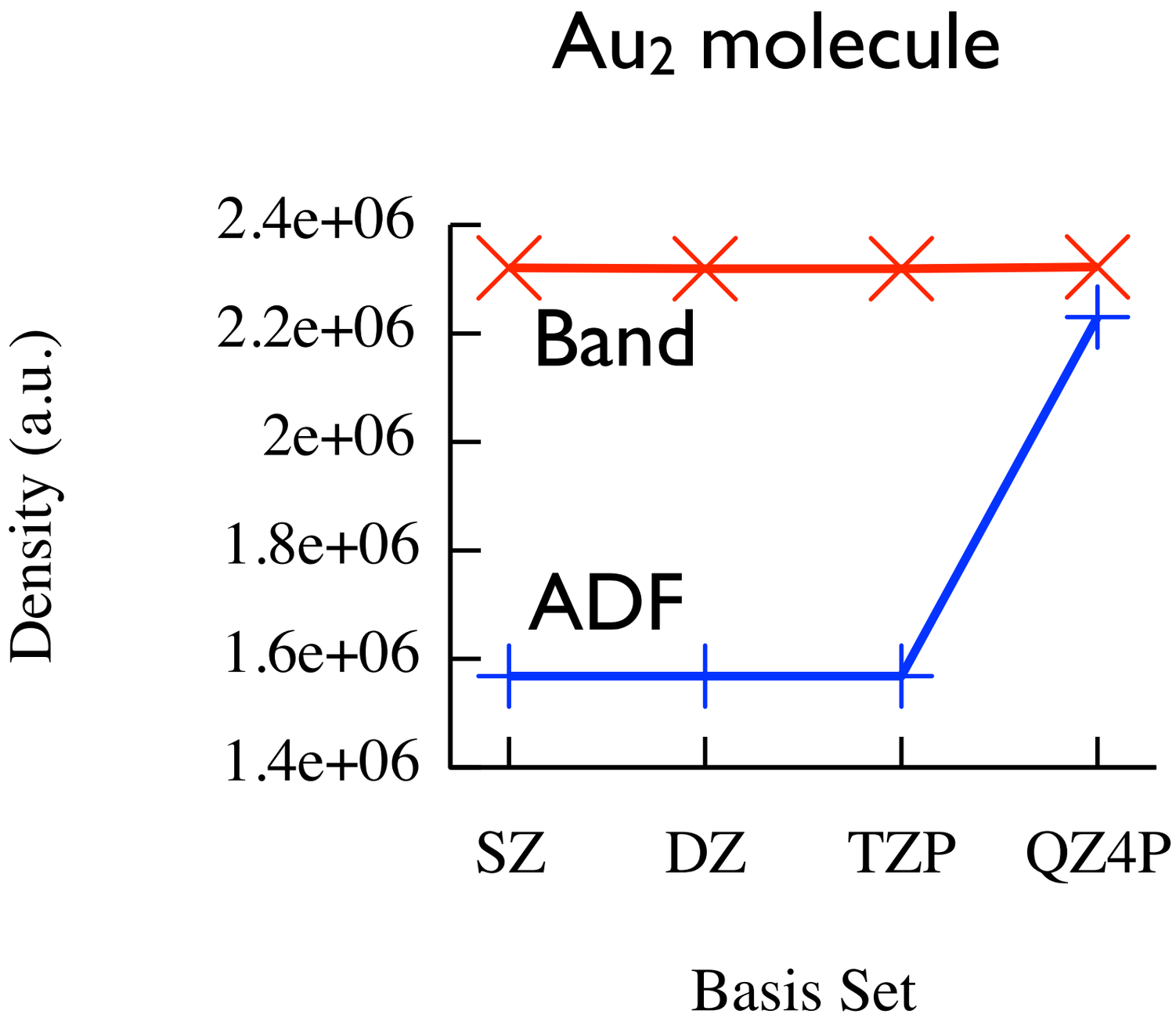
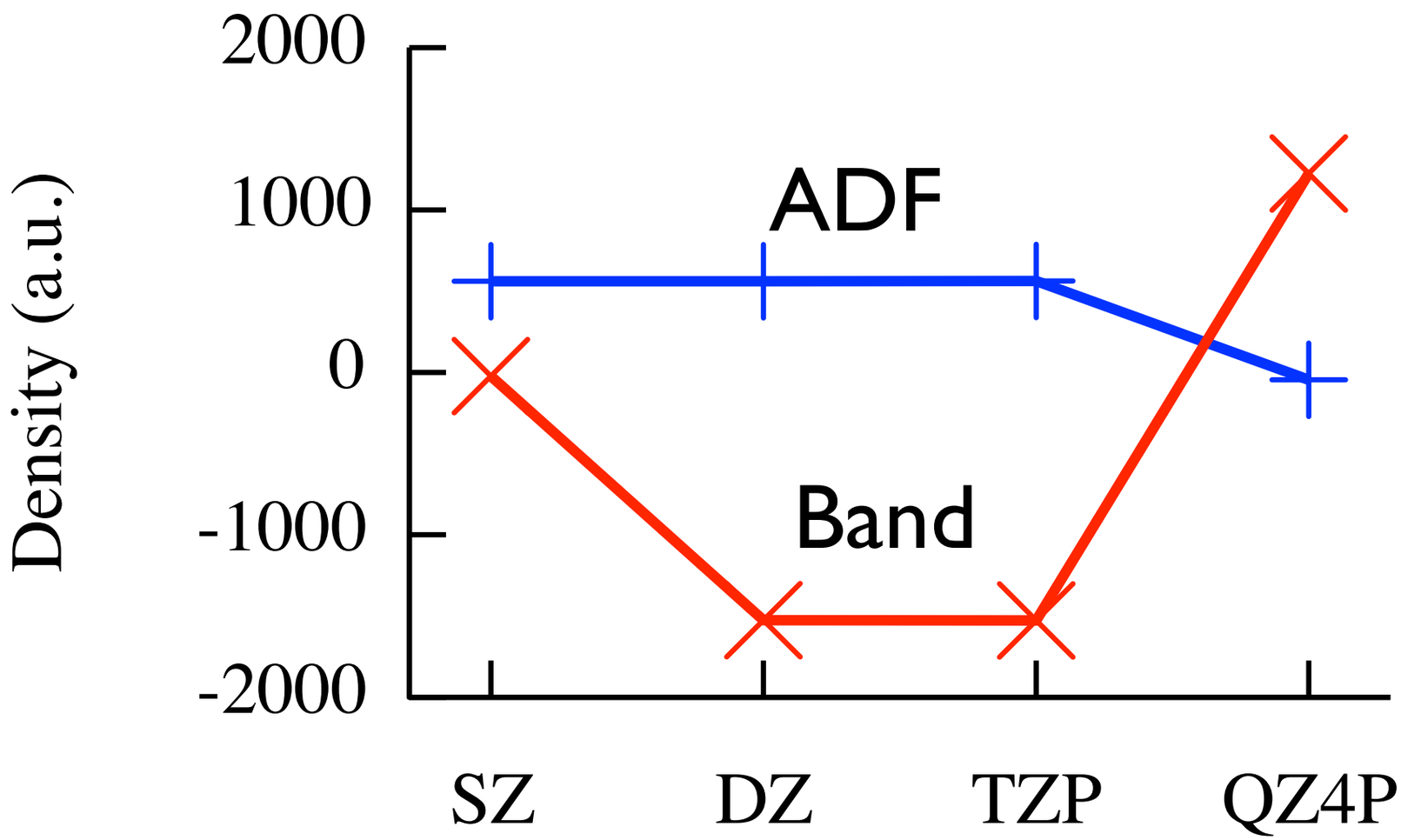


Density change at Nucl.

Of Au in AuH and Au_2 molecule



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  - Better for total energy (not bond energy)
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  - Mixed NAO/STO basis: no panacea (good alternative)

Thank You