

**ATOMISTIC MODELLING OF MATERIALS (MT41028)**  
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**Material:** ZnS is one of the first semiconductors discovered. ZnS has a of applications in optoelectronics (LEDs, displays etc.).

**Question: (4 credit)**

1. Find out the equilibrium lattice constant and bulk modulus of ZnS. An initial guess for the lattice parameter can be 5.3 Å. The input file (zns.scf.in) is attached.

Use the command:

```
pw.exe -in zns.scf.in > output_name
```

Compare your results with published literature (google search). ( 4 credit)