# README

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## Contents



## 1 Purpose

Calculate two-body entropy from pair correlation function.

## 2 Dependency

GSL - GNU Scientific Library is required. In general, it is installed by default in Linux operating systems. Or you can refer to GSL website.

## 3 Compilation

Type "make" and it will generate a "pdf2s2_v2" binary.

## 4 Usage

"pdf2s2_v2 -x XDATCAR" for calculation or "pdf2s2_v2 -h" for help page.

### 4.1 Input files

1. Mass This file contains three rows:
   - type of species.
   - atomic numbers.
   - atomic masses [a.u.] in atomic units.
2. Trun This file contains in value which is the temperature of MD simulation.
3. XDATCAR Standard output of VASP runs.
4. pdf files Pair distribution functions. You can generate those using "pdfxdat" command.

### 4.2 Output files

1. pdf.??.s2 Two-body entropy as a function of integral distance of each kind of pair in a form of

   R [A]  S2(fluct) [kB]  S2(info) [kB]  S2(tot) [kB]

2. tot.s2 Total two-body entropy as a function of integral distance a form of

   R [A]  S2(fluct) [kB]  S2(info) [kB]  S2(tot) [kB]