This article presents the data on a parametric temperature dependent potential for $\beta$-PbF$_2$ using molecular dynamics (MD) simulations in the rigid ion approach. The $\beta$-PbF$_2$ is an important ionic conductor that exhibit a super ionic behavior at 711 K. The understanding of the temperature effect in its properties is crucial for possible applications in electrode for solid state batteries, Cherenkov detectors, and rare earth host for scintillation screen. The simulations were done in the DL_POLY Classic 1.9 package employing the Buckingham pair-potential type. The data have not been reported nor discussed in the research paper to be submitting.

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Most of the bulk properties of fluorite structure ionic crystals, such as CaF$_2$ [4], BeF$_2$ [5], UO$_2$ [3], and PbF$_2$ [6] can be simulated by MD using a Buckingham potential type:

\[ U(r_{ij}) = A_{ij} \exp \left( -\frac{r_{ij}}{\rho_{ij}} \right) - \frac{C_{ij}}{r_{ij}^6} + q_i q_j / r_{ij}, \tag{1} \]

where the first term of the right side is known as the energy repulsion, and represent the electronic overlap, while the second is a well-known dispersion term present in the Lennard-Jones (6–12) potential, which is due to the Coulomb interaction.

In order to modify the $\beta$-PbF$_2$ potential given by eq. (1), the $\rho_{ij}$ coefficient is replaced by a temperature function $\rho_{ij}(T)$, with $i = $ Pb (lead) and $j = $ F (fluorine), respectively. The objective is to find the best $\rho_{ij}(T)$ function, that match well with the experimental lattice parameter data reported in Ref. [7].

Therefore, $\rho_{ij}(T)$ values are presented. All data are shown in Tables 1 and 2. In both tables, the first column are the density values choose in the range from 0.490 to 0.520 eV for the Buckingham fitting parameter, while the second column are computed data of the lattice parameter, $a_0$, obtained using the computer simulation technique of MD.

### Table 1

Lattice parameter for different $\rho_{ij}$ values considering the temperature as a parameter.

| $\rho(T)$ (eV) | Lattice parameter $a_0$ (Å) for different temperatures |
|---------------|-------------------------------------------------------|
|               | 300 K  | 400 K  | 500 K  | 600 K  | 700 K  | 720 K  | 740 K  | 760 K  | 780 K  | 800 K  | 820 K  | 840 K  | 875 K  | 900 K  |
| 0.490         | 5.716  | 5.755  | 5.735  | 5.759  | –      | –      | –      | –      | –      | –      | 5.903  | –      | –      | –      |
| 0.495         | –      | –      | –      | –      | 5.819  | 5.825  | 5.833  | 5.840  | 5.854  | 5.860  | 5.868  | 5.874  | 5.967  | 5.912  |
| 0.500         | 5.798  | 5.823  | 5.853  | 5.878  | 5.920  | 5.930  | 5.939  | 5.944  | 5.954  | 5.967  | 5.976  | 5.978  | 6.003  | 6.025  |
| 0.505         | 5.894  | 5.911  | 5.969  | 5.981  | 6.030  | 6.036  | 6.050  | 6.054  | 6.066  | 6.076  | 6.088  | 6.103  | 6.058  | 6.159  |
| 0.510         | 5.992  | 6.016  | 6.053  | 6.088  | 6.136  | 6.147  | 6.154  | 6.166  | 6.177  | 6.191  | 6.199  | 6.221  | 6.107  | 6.107  |
| 0.516         | 6.110  | 6.142  | 6.181  | 6.211  | –      | –      | –      | –      | –      | –      | 6.121  | –      | –      | –      |
| 0.520         | 6.190  | 6.204  | 6.256  | 6.296  | –      | –      | –      | –      | –      | –      | –      | –      | –      | –      |
2. Experimental design, materials, and methods

2.1. MD simulation detail

The data reported here was obtained using DL_POLY Classic 1.9 package develop by Smith et al. [8] at the Daresbury Laboratory. In this work, the calculations were performed in a cubic simulation box with 768 atoms and long size of 23.720 Å. VESTA [9] was used to prepare the unit cell, while the supercell was created with Atomsk package [10]. Periodic boundary has been used in order to reproduce the bulk properties. The system was previously equilibrated at environmental conditions: 300 K and 1 atm, respectively. In order to compute the crystal expansion (lattice parameters), the simulations were performed in a NVT ensemble and then relaxed into a NPT ensemble, where the number of the ions (N), temperature (T) and pressure (P) are kept constant. A 5 fs integration time is used to find the $\rho(T)$, then a 1 fs integration time is used to performance a new simulation at the $\rho(T)$ correct values, with finality

| $\rho(T)$ (eV) | Lattice parameter $a_0$ (Å) |
|----------------|-----------------------------|
| 0.495          | 5.941                       |
| 0.496          | 5.950                       |
| 0.497          | 5.985                       |
| 0.498          | 6.002                       |
| 0.499          | 6.165                       |
| 0.500          | 6.120                       |

Table 2
Lattice parameter for different $\rho_0$ values at 930 K.

| Atomic pairs | $A_{ij}$ (eV) | $\rho_{ij}$ (Å) | $C_{ij}$ (eV Å$^6$) |
|--------------|---------------|-----------------|---------------------|
| Pb – Pb      | 0.0           | 0.0             | 0.0                 |
| Pb – F       | 122.7         | Tab. 1–2        | 107.3               |
| F – F        | 10255         | 0.225           | 107.3               |

Table 3
Adjustment constants of the potentials that describe the β-PbF$_2$ by MD [11].

Fig. 1. Values for the adjustment parameter $\rho(T)$ as a function of temperature.
to corroborate the accurate lattice parameter at each temperature. In both cases, a 10 Å cutoff is employed, and the Ewald sum is used to compute the Coulomb long range potential. The used potential parameters are summarized in Table 3. The data is obtained from Walker et al. [11] as well the modifications proposed in the Section 1.

2.2. Parametric temperature dependent potential for $\beta$-PbF$_2$

From the Tables 1 and 2 a linear fitting is done for each temperature. In order to find the better lattice parameter value, thermal expansion measurements for PbF$_2$ obtained by Goff et al. [7] by neutron diffraction at different temperatures were employed. The $\rho(T)$ values are shown in Fig. 1.

In order to make a first approximation on the validation of the potential data shown in Fig. 1, the enthalpy of the atomic system was recorded (refer to Table 4).

**Table 4**

| Temperature (K) | Enthalpy (kJ mol$^{-1}$) |
|----------------|--------------------------|
| 300            | -2239.19618              |
| 350            | -2236.83185              |
| 370            | -2235.87824              |
| 400            | -2234.44629              |
| 420            | -2233.46642              |
| 450            | -2231.99567              |
| 470            | -2230.98597              |
| 500            | -2229.42186              |
| 520            | -2228.37485              |
| 550            | -2226.68132              |
| 570            | -2225.5548               |
| 600            | -2223.77367              |
| 620            | -2222.5076               |
| 650            | -2220.55895              |
| 670            | -2219.266                |
| 700            | -2217.2881               |
| 720            | -2215.84356              |
| 750            | -2213.80256              |
| 770            | -2212.31626              |
| 800            | -2210.2459               |

**Fig. 2.** The enthalpy for $\beta$-PbF$_2$. In filled square, data obtained by MD; in solid line, the linear fit.
The specific heat capacity at constant pressure, \( C_p \), is calculated from Table 4 and the slope of the linear fit shown in Fig. 2. The \( C_p \) value obtained by MD is \( 58 \pm 1 \text{ J mol}^{-1} \text{ K}^{-1} \) which is in acceptable agreement with reported value of \( 69 \pm 7 \text{ J mol}^{-1} \text{ K}^{-1} \) between 400 and 640 K [12].

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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