pair_style coul/debye/vk command

Syntax

```
pair_style coul/debye/vk global_cutoff
pair_coeff i j kappa cutoff
```

- global_cutoff = global cutoff for Debye-shielded Coulombic interactions
- i, j = atom types
- kappa = (inverse) Debye length
- cutoff = (optional) cutoff between individual pairs

Examples

```
pair_style coul/debye/vk 5.0
pair_coeff * * 1.0

pair_style coul/debye/vk 5.0
pair_coeff 1 1 1.0
pair_coeff 2 2 2.0 2.5
```

Description

The style *coul/debye/vk* adds an additional exp() damping factor to the Coulombic term, given by

$$E = \frac{Cq_iq_j}{\epsilon r}\exp(-\kappa_{ij}r) \quad r < r_{c,ij}\,, \qquad (1)$$

where C is an energy-conversion constant, q_i and q_j are the charges on the 2 atoms, and ϵ is the dielectric constant which can be set by the dielectric command. The cutoff $r_{c,ij}$ truncates the interaction distance.

Notice that this style differs from *coul/debye* in the Debye screening length: the inverse Debye screening length κ is a global parameter in *coul/debye*, i.e. it applies for all pairs, whereas in *coul/debye/vk*, each pair is assigned with an individual κ_{ij} value.

At least all the κ_{ij} values for i = j need to be set; for i != j, the inverse screening length can be automatically obtained by applying mixing rules. The default mixing rule is *geometric*, i.e. $\kappa_{ij} = \sqrt{\kappa_{ii}\kappa_{jj}}$.

The cutoff parameter in pair_coeff command is optional. If it is not used (as in some of the examples above), the default global value specified in the pair_style command is used.

Mixing, shift, table, tail correction, restart, rRESPA info

For atom type pairs i,j and i != j, the cutoff distance and kappa can be mixed. The default mix value for both are *geometric*. See the "pair_modify" command for details.

The pair_modify shift option is not relevant for these pair styles.

This pair style do not support the pair_modify tail option for adding long-range tail corrections to energy and pressure.

These pair styles write their information to binary restart files, so pair_style and pair_coeff commands do not need to be specified in an input script that reads a restart file.

These pair styles can only be used via the *pair* keyword of the run_style respa command. They do not support the *inner*, *middle*, *outer* keywords.