List of files that were changed:

Original version: 03_18_2024 (cloned from RASPA2 master repository on Github)

Modified version (this version): 04_30_2024 (uploaded to Manz Group fork on Github)

Changes that have been successfully tested are marked in blue.

file name	function name	note
framework.c	-	• Defining a case for the new bending potential (MANZ_BEND) and converting the input parameters (i.e., from kelvin to energy and from degree to radians) • Defining four cases for the new torsion potentials (i.e., CADT_MODE_ONE_ONLY, CADT_DIHEDRAL, ADDT_MODE_ONE_ONLY, and ADDT_DIHEDRAL) and converting the input parameters (i.e., from kelvin to energy and from degree to radians)
framework_energy.c	CalculateFrameworkBendEnergy	Defining a case for MANZ_BEND potential to calculate the bend potential (U) value.
	CalculateFrameworkTorsionEnergy	Defining four cases for new torsion potentials (i.e., CADT_MODE_ONE_ONLY, CADT_DIHEDRAL, ADDT_MODE_ONE_ONLY, and ADDT_DIHEDRAL) to calculate the torsion potential (U) values.
framework_force.c	CalculateFrameworkBendForce	Defining a case for MANZ_BEND potential to calculate the bend potential (U) value and the first derivate of bend potential (defined as DF in the code).
	CalculateFrameworkTorsionForce	• Defining four cases for new torsion potentials (i.e., CADT_MODE_ONE_ONLY, CADT_DIHEDRAL, ADDT_MODE_ONE_ONLY, and ADDT_DIHEDRAL) to

		calculate the torsion potential (U) values. • Defining two new approaches to calculate forces for CADT and ADDT cases.
framework_hessian.c	ComputeFrameworkBendHessian	Defining a case for MANZ_BEND potential to calculate the bend potential (U) value and the first and second derivates of bend potential (defined as DF and DDF in the code respectively).
	ComputeFrameworkTorsionHessian	• Displacement of the atom in the linear bond angle • Defining four cases for new torsion potentials (i.e., CADT_MODE_ONE_ONLY, CADT_DIHEDRAL, ADDT_MODE_ONE_ONLY, and ADDT_DIHEDRAL) to calculate the torsion potential (U) values and first and second derivatives of torsion potentials (DF and DFF). **Note:** Only DF and DFF are going to be calculated for CADT cases. For ADDTs, they are going to be developed in future versions.
framework_born.c	CalculateFrameworkBendBornTerm	Defining a case for MANZ_BEND potential to calculate the bend potential (U) value and the first and second derivates of bend potential (defined as DF and DDF in the code respectively).
	CalculateFrameworkBendBornTerm	• Displacement of the atom in the linear bond angle • Defining four cases for new torsion potentials (i.e., CADT_MODE_ONE_ONLY, CADT_DIHEDRAL, ADDT_MODE_ONE_ONLY, and ADDT_DIHEDRAL) to calculate the torsion potential (U) values and first and second derivatives of torsion potentials (DF and DFF).

		Note: Only DF and DFF are going to be calculated for CADT cases. For ADDTs, they are going to be developed in future versions.
internal_energy.c	CalculateBendEnergy	Defining a case for MANZ_BEND potential to calculate the bend potential (U) value.
	CalculateBendEnergyAdsorbate	
	CalculateBendEnergyCation	
	CalculateTorsionEnergy	Defining four cases for new torsion potentials (i.e., CADT_MODE_ONE_ONLY, CADT_DIHEDRAL, ADDT_MODE_ONE_ONLY, and ADDT_DIHEDRAL) to calculate the torsion potential (U) values.
	CalculateTorsionEnergyAdsorbate	
	CalculateTorsionEnergyCation	
internal_force.c	CalculateAdsorbateBendForce	Defining a case for MANZ_BEND potential to calculate the bend potential (U) value and the first derivate of bend potential (defined as DF in the code).
	CalculateCationBendForce	
	CalculateAdsorbateTorsionForce	• Defining four cases for new torsion potentials (i.e., CADT_MODE_ONE_ONLY, CADT_DIHEDRAL, ADDT_MODE_ONE_ONLY, and ADDT_DIHEDRAL) to calculate the torsion potential (U) values. • Defining two new approaches to calculate forces for CADT and ADDT cases.
	CalculateCationTorsionForce	
internal_hessian.c	CalculateAdsorbateBendHessian	Defining a case for MANZ_BEND potential to calculate the bend potential (U) value and the first and second derivates of bend potential (defined as DF and DDF in the code respectively).
	CalculateCationBendHessian	
	CalculateAdsorbateTorsionHessian	• Displacement of the atom in the linear bond angle • Defining four cases for new torsion potentials (i.e., CADT_MODE_ONE_ONLY, CADT_DIHEDRAL, ADDT_MODE_ONE_ONLY, and ADDT_DIHEDRAL) to
	CalculateCationTorsionHessian	

		calculate the torsion potential (U) values and first and second derivatives of torsion potentials (DF and DFF). **Note:** Only DF and DFF are going to be calculated for CADT cases. For ADDTs, they are going to be developed in future versions.
internal_born.c	CalculateAdsorbateBendBornTerm	Defining a case for MANZ_BEND potential to calculate the bend potential (U) value and the first and second derivates of bend potential (defined as DF and DDF in the code respectively).
	CalculateCationBendBornTerm	
	CalculateAdsorbateTorsionBornTerm	• Displacement of the atom in the linear bond angle • Defining four cases for new torsion potentials (i.e., CADT_MODE_ONE_ONLY, CADT_DIHEDRAL, ADDT_MODE_ONE_ONLY, and ADDT_DIHEDRAL) to calculate the torsion potential (U) values and first and second derivatives of torsion potentials (DF and DFF). **Note:** Only DF and DFF are going to be calculated for CADT cases. For ADDTs, they are going to be developed in future versions.
	CalculateCationTorsionBornTerm	
alchemical_transformation.c	AllocateTransientComponentMemory	Defining MANZ_BAND case and assigning values to each parameter.
		Defining all four new torsion type cases (CADT_MODE_ONE_ONLY, CADT_DIHEDRAL, ADDT_MODE_ONE_ONLY, and ADDT_DIHEDRAL) and assigning values to their parameters.
status.c	PrintBendEnergyStatus	Defining MANZ_BEND case to calculate new bend potential (U) and print the input parameters and the bend potential (U) values.
	PrintTorsionEnergyStatus	Defining all four new torsion type cases (CADT_MODE_ONE_ONLY, CADT_DIHEDRAL, ADDT_MODE_ONE_ONLY, and

		ADDT_DIHEDRAL) to calculate torsion potentials and print the input parameters and the bend potential (U) values for each case separately.
molecule.c	ReadComponentDefinition	Defining MANZ_BEND case and convert the input parameters.
		Defining all four new torsion type cases (CADT_MODE_ONE_ONLY, CADT_DIHEDRAL, ADDT_MODE_ONE_ONLY, and ADDT_DIHEDRAL) and convert the input parameters for each one of them.
output.c	PrintPreSimulationStatusCurrentSystem	Defining MANZ_BEND case and print the converted input parameters.
		Defining all four new torsion type cases (CADT_MODE_ONE_ONLY, CADT_DIHEDRAL, ADDT_MODE_ONE_ONLY, and ADDT_DIHEDRAL) and print the converted input parameters.
potentials.c	-	Adding MANZ_BEND to the list of BendTypes (i.e., {2,"MANZ_BEND"}).
		Adding all four new torsion potential cases to the list of TorsionTypes (i.e., {2,"CADT_MODE_ONE_ONLY"}, {8,"CADT_DIHEDRAL"}, {4,"ADDT_MODE_ONE_ONLY"}, {10,"ADDT_DIHEDRAL"})
potentials.h	-	Adding MANZ_BEND to the list of bend types and changing NR_BEND_TYPES value to match the number of bend types.
		Adding CADT_MODE_ONE_ONLY, CADT_DIHEDRAL, ADDT_MODE_ONE_ONLY, and ADDT_DIHEDRAL to list of torsion types and changing NR_TORSION_TYPES value to match the number of torsion types.
constants.h	-	Defining new constants.

Notes:

(1) New angle-bending potential: The equation for Manz_bend is

$$U_{new}[\theta] = \frac{2\left(\cos\theta - \cos\theta_{eq}\right)^2}{\sin^2\theta + 3\sin^2\theta_{eq}\left(\frac{\tanh\left[2\sin\left[\theta/2\right]\right]}{\tanh\left[2\sin\left[\theta_{eq}/2\right]\right]}\right)} \quad (1)$$

The energies and forces have been programmed for this new potential. Tests of the energies and forces were performed for the framework atoms using the 'Numerical' simulation type which compares analytic to numerically-computed (finite difference method) forces. Programmed but not yet tested for the molecules. The Hessian and elastic constant terms have been programmed but not tested.

(2) New dihedral potentials: Constant amplitude dihedral torsion (CADT) and angle-damped dihedral torsion (ADDT). CADT_MODE_ONE_ONLY has only the first torsion mode with no bond angle damping. CADT_DIHEDRAL includes all seven torsion modes with no bond angle damping. ADDT_MODE_ONE_ONLY has only the first torsion mode with bond angle damping. ADDT_DIHEDRAL includes all seven torsion modes with bond angle damping. The energies and forces have been programmed for all four of these new dihedral torsion potentials. Tests of the energies and forces were performed for the framework atoms using the 'Numerical' simulation type which compares analytic to numerically-computed (finite difference method) forces. Programmed but not yet tested for the molecules. For CADT mode 1 and CADT dihedral, the Hessian and elastic constant terms have been programmed but not tested. For ADDT mode 1 and ADDT dihedral, the Hessian and elastic constant terms have not been programmed.

(3) There is a folder named tests_and_examples that contains examples using these new potentials. Each subfolder inside this folder contains the input files and a copy of the main output file (results).

(4) We have submitted two journal manuscripts (currently under review) that contain the detailed equations and their derivations for these new angle-bending and dihedral-torsion potentials.