

Insights on the robustness, sensitivity and expressivity of simple many-body potentials: application to α -Zr

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May 2022



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INITIATIVE D'EXCELLENCE

Atomic-scale modelling

DFT (*Density Functional Theory*)

- Approx. solution of Schrödinger equation
- Precision
- Limited to small-sized simulation boxes
- **High computational cost**

Potentials

- ML and classical interatomic potentials
- Less accurate
- Efficient predictions of energy and forces
- **Computationally affordable methods**

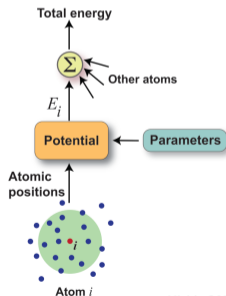
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Mishin 2021

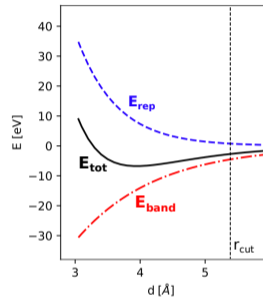
Classical interatomic potentials

- EAM, MEAM...
- Based on a **physical understanding** of interatomic bonding in the material
- Reasonable transferability
- Less flexible than ML potentials (Mishin 2021)
- **Computationally light**

Second Moment Approximation (SMA) potential (close to EAM - Finnis Sinclair potential)

$$E_i^{tot} = -\xi \sqrt{\sum_{j \neq i}^{r_{cut}} e^{-2q(\frac{r_{ij}}{r_0} - 1)}} + A \sum_{j \neq i}^{r_{cut}} e^{-p(\frac{r_{ij}}{r_0} - 1)}$$

- Non-linear many-body potential, used for metals (Finnis & Sinclair 1984)
- **4 parameters** $\theta = \{p, q, A, \xi\}$
- Cutoff radius $r_{cut} \rightarrow$ range
- Identification of parameters $\theta \rightarrow$ crucial (but challenging)

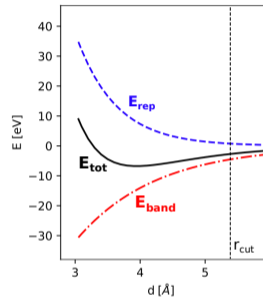


Effect of parameters on computed properties ?

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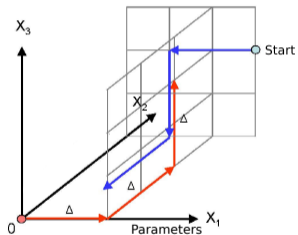
Material context: zirconium

- Nuclear fuel cladding material (Zircaloy)
- Irradiation \Rightarrow **Vacancy and SIAs defects**
- Defect diffusion & clustering related to irradiation growth

Objectives

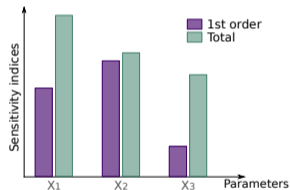
Robustness

- Model screening



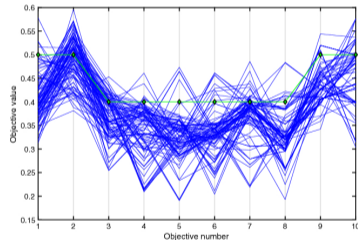
Sensitivity

- Variance-based sensitivity indices



Expressivity

- Multi-objective optimization



Used SMA potentials

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- Parameters: $\theta = \{p, q, A, \xi\}$
- Range: r_{cut}

Dufresne potential (2015)

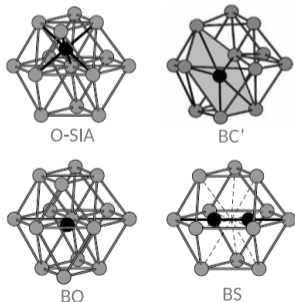
- **Short range:** between 2nd – 3rd neighbours
- Fitted on bulk properties of *fcc* Zr at 0K
- $\theta_D = \{7.376, 2.492, 0.269, 2.693\}$
- SIAs defects and stacking faults not well described

Willaime potential (1991)

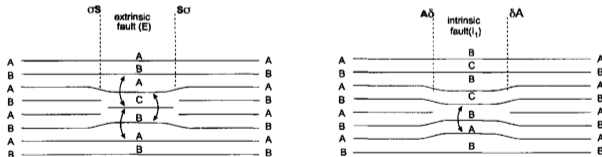
- **Medium range:** between 6th – 7th neighbours
- Fitted on bulk properties of *hcp* Zr at 0K
- $\theta_W = \{9.3, 2.1, 0.179, 2.201\}$
- SIAs defects and stacking faults not well described

Quantities of interest (QOIs)

- Structure: $a, \frac{\epsilon}{a}, E_c$
- Elastic properties: C_{ij}
- Formation energy of point defects: *Vacancy, SIAs*
- Stacking faults energies: γ_{SF} (prismatic + basal)



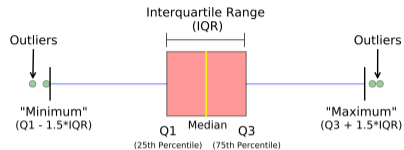
SIAs defects, V \acute{e} rit \acute{e} et al., Phys. Rev. B, 87 (2013)



Stacking faults in hcp lattice, Hull & Bacon (2001)

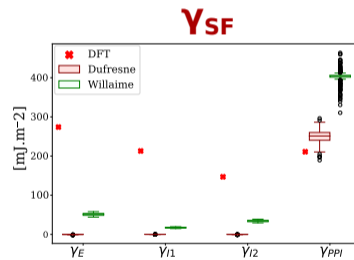
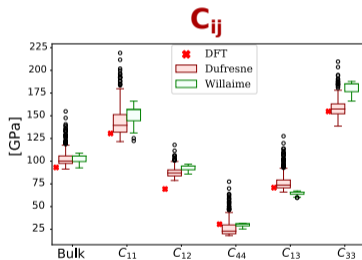
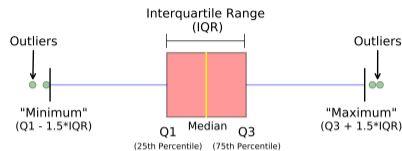
Screening

- 2.5% variation around the fitted parameters sets θ_D and θ_W
- Uniform distributions (assumption)
- Nominal r_{cut}



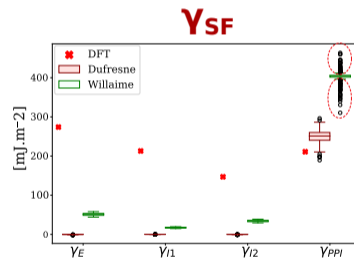
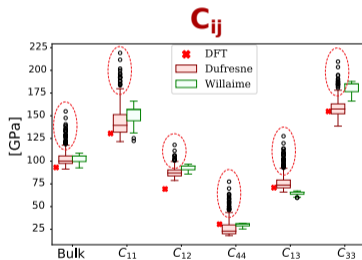
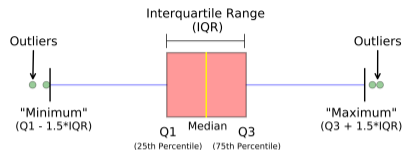
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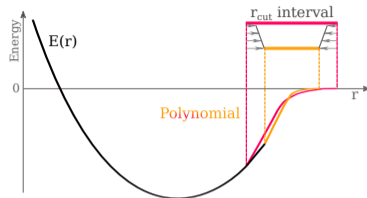
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- Outliers, asymmetry... especially on C_{ij}
- Strong effect on small range potential
- Role of the cutoff? *i.e.* role of strong gradient zones?

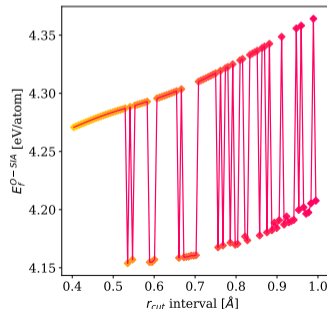
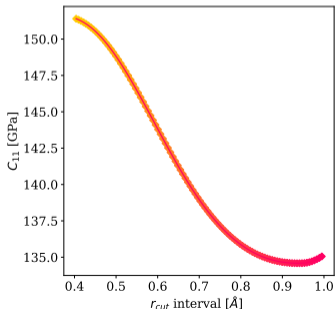
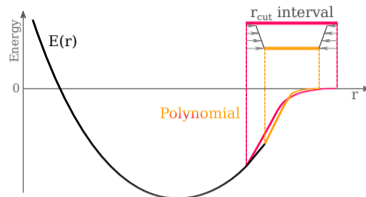
Effect of the cutoff handling

- 30% variation inside the **cutoff interval** $r_{cut} = [r_{cut}^i, r_{cut}^e]$



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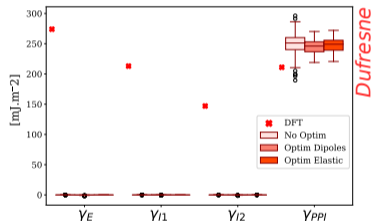
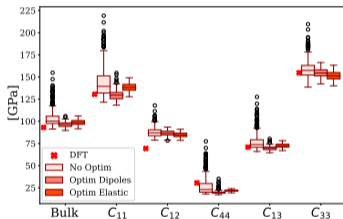
- 30% variation inside the **cutoff interval** $r_{cut} = [r_{cut}^i, r_{cut}^e]$
- Strong effect on properties
- Complex mapping r_{cut} interval / properties
- Need to find the "good" r_{cut} interval for each random parameters set



Reduction of the artefacts

Optimization of the cutoff interval

- $\forall \theta_i \rightarrow r_{cut}$ interval $\{(C_{ij}, E_f, \gamma)\}$ are stable
- C_{ij} or P_{ij} based strategy (*Optim Elastic* or *Optim Dipoles*)

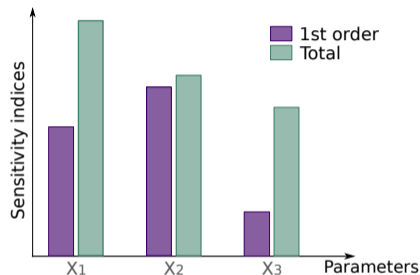


- Reduction of artefacts \Rightarrow improved robustness
- Need to take care of the r_{cut} interval for:
 - implementing a potential into MD codes and get correct values
 - sensitivity analysis \Rightarrow **avoid non-physical values** (cf. Dhaliwal et al. 2019)

Sobol's method

Sobol, Math. Model. Comput. Exp. , 407 (1993)

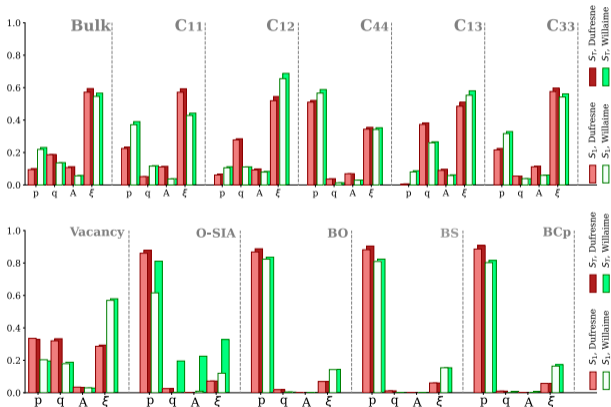
- **First order indices:** $S_i = \frac{V_i}{V_Y}$
- Higher order indices: $S_{ij} = \frac{V_{ij}}{V_Y}$, $S_{ijk} = \frac{V_{ijk}}{V_Y}$, ...
- **Total indices:** $S_{T_i} = S_i + S_{ij} + S_{ijl} + \dots + S_{i\dots k}$
- N.B.: $(S_{T_i} - S_i) \Rightarrow$ influence of the interactions between parameters



This work

- 2.5% variation around the fitted parameters sets θ_D and θ_W
- Uniform distributions (assumption)
- Stratified latin hypercube sampling
- Sampled sets: $\theta_i, i = 1 \dots N \times (2^k)$, with $N = 500$ and $k = 4$ parameters
- Optimized r_{cut} interval

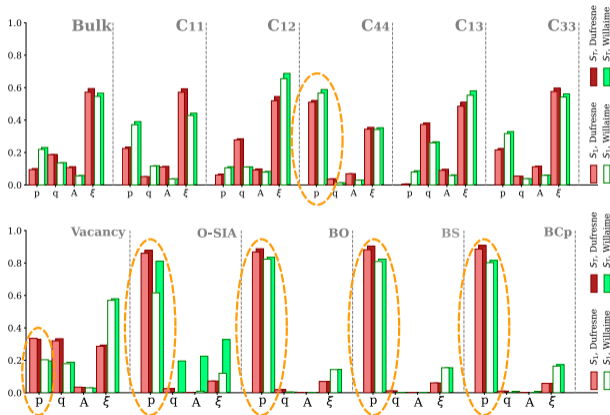
Results



This work

- $S_i \approx S_T$ for C_{ij} and E_f
- **p**:
 - Strong effect on E_f^{SIAs}
 - Moderate effect on $E_f^{Vacancy}$ and C_{ij} (except C_{44})
- **ξ**:
 - Strong effect on C_{ij}
 - Rather important on $E_f^{Vacancy}$

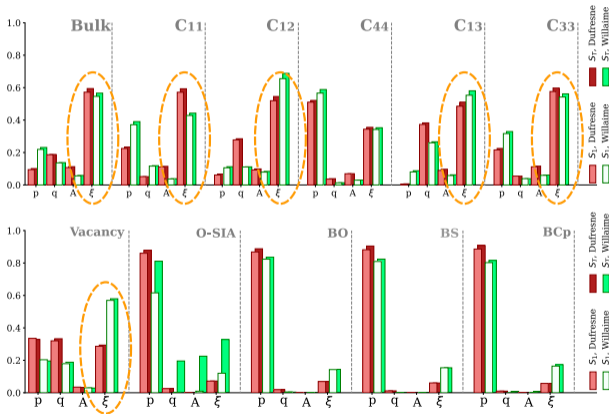
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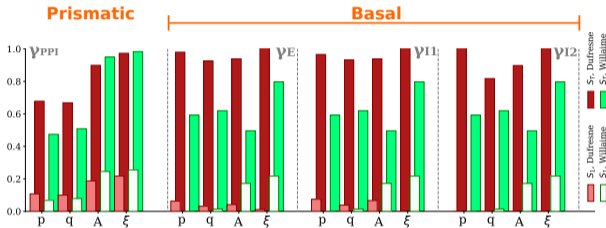
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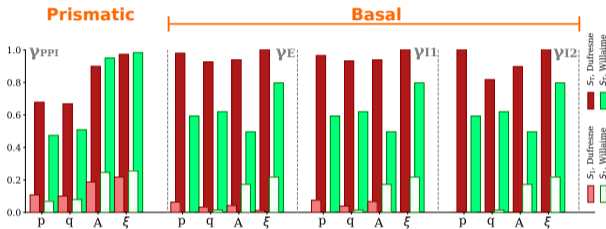
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- γ_{SF} :
 - Similar indices for I_1 , I_2 and E faults (Hirth & Lothe 1982)
 - Effects of parameters are indirect
 - Fairly high influence of (p, ξ) interaction.

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 - Effects of parameters are indirect
 - Fairly high influence of (p, ξ) interaction.
- Sensitivity indices can guide potential fitting

Metamodel and multi-objective optimization

Polynomial chaos-based metamodel (Ghanem et al., J. Appl. Mech. 57 (1990))

- PCE-based **surrogate model** for a , c/a , C_{ij} and E_f (**with correction of artefacts**):

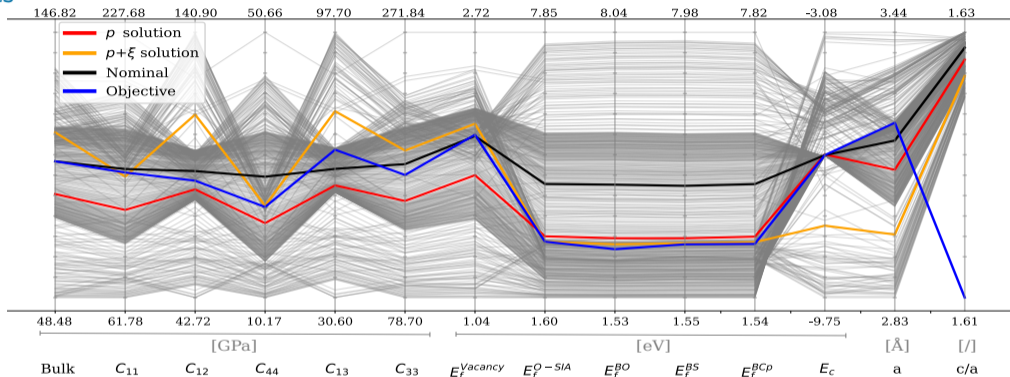
$$Y = \sum_{\alpha} y_{\alpha} \Psi_{\alpha}(\theta)$$

- Legendre polynomials (suited for uniform distributions of parameters)
- only p and (p, ξ) parameters used to build the model
- $p=[7, 13.94]$, $\xi=[0.42, 3]$, $A=0.17936$, $q=2.1$ (based on *Willaime* potential)

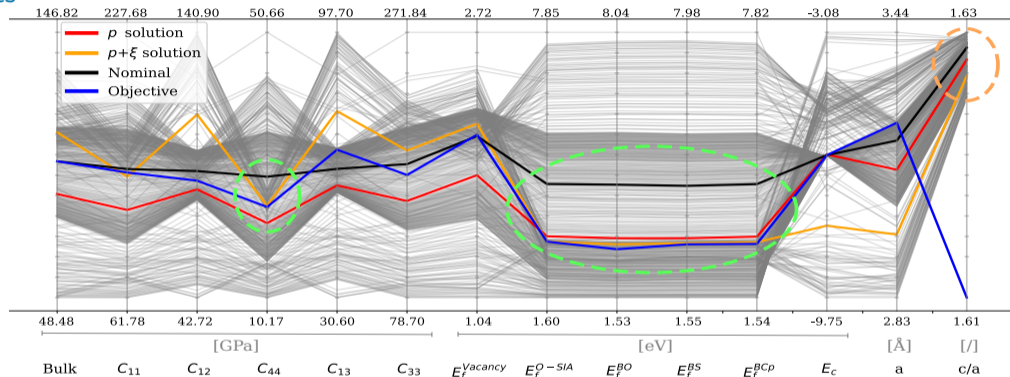
Multi-objective optimization

- Non-dominated sorting genetic algorithm II (*NSGA-II*) (Deb et al., IEEE Trans. Evol. Comput. 6, 182 (2002))
- Genetic algorithm with a modified mating and survival selection
- *pymoo* implementation (Blank and Deb, IEEE Access 8, 89497 (2020))
- **Objective function**: DFT reference values for a , c/a , C_{ij} and E_f (14 objectives, same weights)

Results



Results



- Improvement of the formation energies E_f of SIAs point defects and C_{44}
- Ideal c/a
- p solution = 8.04, (p, ξ) solution = (7.513, 2.627)

Results

	Ref.	Optim $p + \xi$	EAM #3	EAM #2		Ref.	Optim $p + \xi$	EAM #3	EAM #2
[GPa]					[eV]				
$Bulk$	99	109.01	99.3	100.2	E_f^V	2.07	2.14	1.67	2.26
C_{11}	140	133.24	142	149	E_f^{O-SIA}	2.915	3.04	2.96	3.13
C_{12}	86	108.86	75	82	E_f^{BO}	2.72	2.837	2.79	2.87
C_{44}	24	24.31	44	48	E_f^{BS}	2.839	2.87	2.93	3.21
C_{13}	68	77.8	76	65	E_f^{BCp}	2.81	2.84	2.88	3.13
C_{33}	168	185.7	168	180	E_f^{2Va}	0.176	0.259	-0.009	0.3
					E_i^{2Vb}	0.094	0.33	0.0069	0.31
	Ref.	Optim $p + \xi$	EAM #3	EAM #2		Ref.	Optim $p + \xi$	EAM #3	EAM #2
E_c [eV]	-6.17	-7.94	-6.63	-6.469	[mJm^{-2}]	147	29.61	99	55
a [Å]	3.23	2.98	3.23	3.22	γ_{I1}	213	59.21	198	110
$\frac{c}{a}$ []	1.6	1.627	1.59	1.619	γ_{I2}	274	88.8	297	164
$\Delta E_{bcc-hcp}^a$	0.071	0.018	0.054	0.052	γ_E	211	332.21	135	357
$\left[\frac{eV}{atom}\right]$					γ_{PPI}				

– Not perfect C_{ij} (except C_{44})

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- Stacking fault energies not well reproduced → link with c/a ratio and expressivity limit of this SMA with r_{cut} 6 nearest neighbours

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- $E_f^{BO} < E_f^{BCp} < E_f^{BS} < E_f^{O-SIA}$, as in DFT, and in contrast with EAM#2

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C_{13}	68	77.8	76	65	E_f^{BCp}	2.81	2.84	2.88	3.13
C_{33}	168	185.7	168	180	E_i^{2Va}	0.176	0.259	-0.009	0.3
					E_i^{2Vb}	0.094	0.33	0.0069	0.31
	Ref.	Optim $p + \xi$	EAM #3	EAM #2	[$mJ.m^{-2}$]	Ref.	Optim $p + \xi$	EAM #3	EAM #2
E_c [eV]	-6.17	-7.94	-6.63	-6.469	γ_{I1}	147	29.61	99	55
a [Å]	3.23	2.98	3.23	3.22	γ_{I2}	213	59.21	198	110
$\frac{c}{a}$ []	1.6	1.627	1.59	1.619	γ_E	274	88.8	297	164
$\Delta E_{bcc-hcp}^a$	0.071	0.018	0.054	0.052	γ_{PPI}	211	332.21	135	357
$\left[\frac{eV}{atom}\right]$									

- Not perfect C_{ij} (except C_{44})
- Not perfect lattice parameter a and cohesive energy E_c , but hcp more stable than bcc
- Stacking fault energies not well reproduced → link with c/a ratio and expressivity limit of this SMA with r_{cut} 6 nearest neighbours
- $E_f^{BO} < E_f^{BCp} < E_f^{BS} < E_f^{O-SIA}$, as in DFT, and in contrast with EAM#2
- Positive 1nn vacancy binding energies as in DFT, and in contrast with EAM#3

Results

	Ref.	Optim $p + \xi$	EAM #3	EAM #2		Ref.	Optim $p + \xi$	EAM #3	EAM #2
[GPa]					[eV]				
$Bulk$	99	109.01	99.3	100.2	E_f^V	2.07	2.14	1.67	2.26
C_{11}	140	133.24	142	149	E_f^{O-SIA}	2.915	3.04	2.96	3.13
C_{12}	86	108.86	75	82	E_f^{BO}	2.72	2.837	2.79	2.87
C_{44}	24	24.31	44	48	E_f^{BS}	2.839	2.87	2.93	3.21
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	Ref.	Optim $p + \xi$	EAM #3	EAM #2	[mJm^{-2}]	Ref.	Optim $p + \xi$	EAM #3	EAM #2
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- Positive 1nn vacancy binding energies as in DFT, and in contrast with EAM#3
- Refitted potential = good compromise

Conclusions

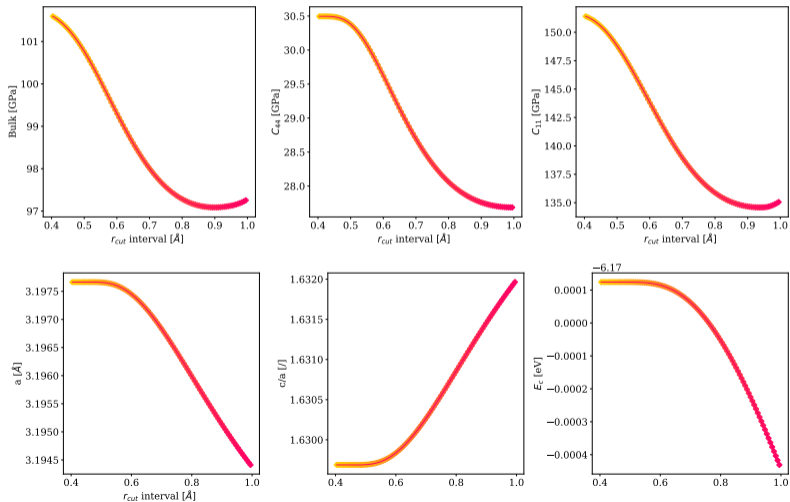
- The robustness of a potential is affected by the existence of strong gradients;
- **A sensitivity indices-oriented technique to refit interatomic potentials is proposed;**
- An **improved SMA potential** is identified, that can be used to study **small point defects physics in α -Zr.**

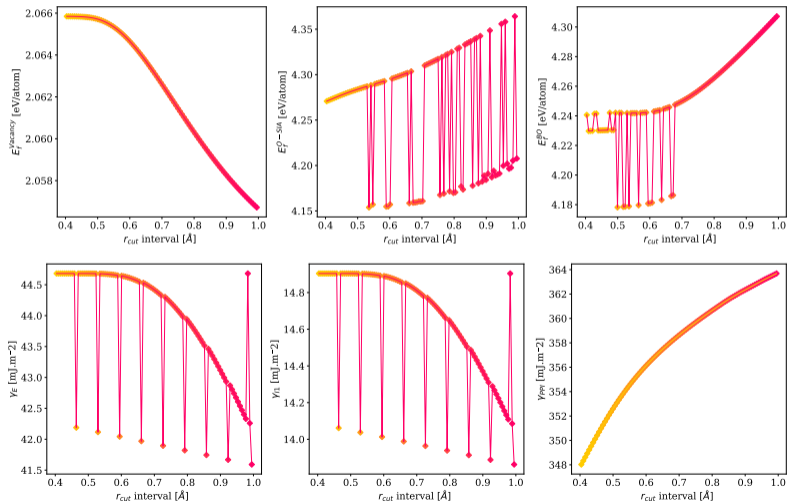
Perspectives

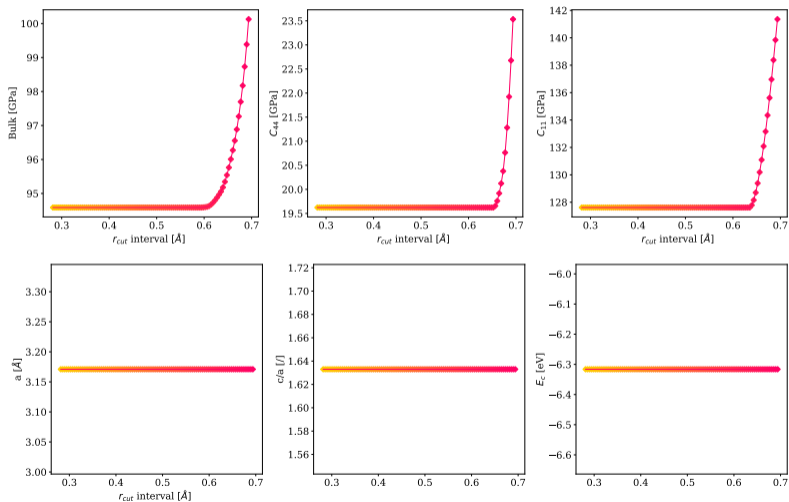
- Application to N-moments TB potentials
- Further efforts to obtain a better SMA potential require:
 - r_{cut} = adjustable parameter (explicitly);
 - a more global SMA model screening, in order to push the optimization problem up to the SMA expressivity limits.

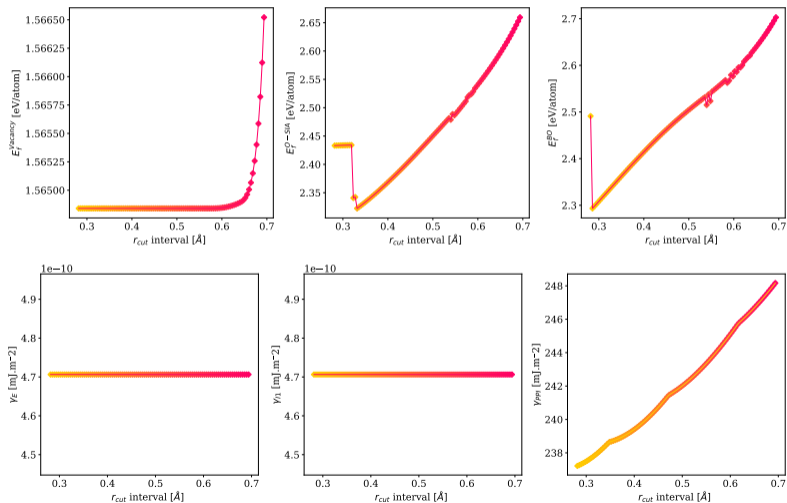
Thank you for your attention.

Properties vs cutoff interval - *Willaime* potential

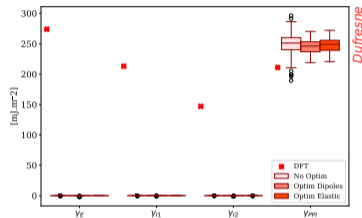
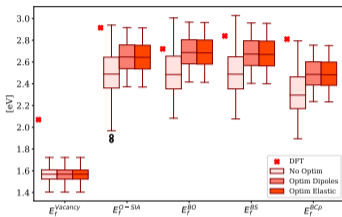
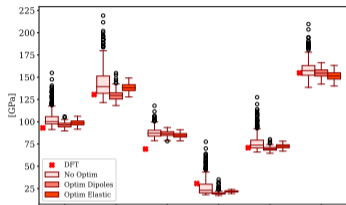


Properties vs cutoff interval - *Willaime* potential

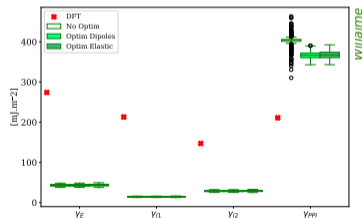
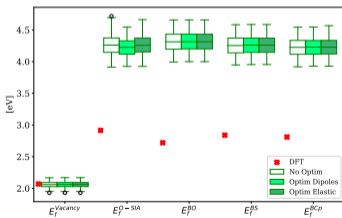
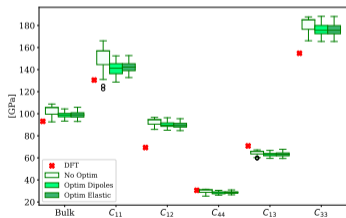
Properties vs cutoff interval - *Dufresne* potential

Properties vs cutoff interval - *Dufresne* potential

Reduction of cutoff effect

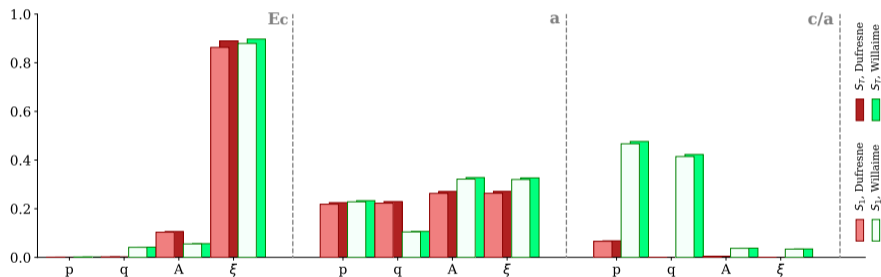


Dufresne



willaime

Sensitivity analysis - lattice parameters



Refitted potential

	Ref.	Nom.	Optim p	Optim $p + \xi$	EAM #3	EAM #2		Ref.	Nom.	Optim p	Optim $p + \xi$	EAM #3	EAM #2
[GPa]							[eV]						
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C_{44}	24	28.62	21.6	24.31	44	48	E_f^{BS}	2.839	4.26	2.981	2.87	2.93	3.21
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C_{33}	168	175.84	148.95	185.7	168	180	E_i^{2Va}	0.176	0.216	0.193	0.259	-0.009	0.3
							E_i^{2Vb}	0.094	0.228	0.219	0.33	0.0069	0.31
	Ref.	Nom.	Optim p	Optim $p + \xi$	EAM #3	EAM #2		Ref.	Nom.	Optim p	Optim $p + \xi$	EAM #3	EAM #2
							[$mJ.m^{-2}$]						
E_c [eV]	-6.17	-6.19	-6.15	-7.94	-6.63	-6.469	γ_{I1}	147	9.93	17.03	29.61	99	55
a [\AA]	3.23	3.19	3.35	2.98	3.23	3.22	γ_{I2}	213	19.86	34.05	59.21	198	110
$\frac{c}{a}$ [/]	1.6	1.63	1.629	1.627	1.59	1.619	γ_E	274	29.79	51.08	88.8	297	164
$\Delta E_{bcc-hcp}^a$	0.071	0.027	0.013	0.018	0.054	0.052	γ_{PPI}	211	367.48	292.85	332.21	135	357
$\left[\frac{eV}{atom}\right]$													