Electronic supplementary material Table 1: Fit parameters of the zinc EAM potential. The parameters of Eq. 10 can be calculated from $F'(\rho_e)$ and $F''(\rho_e)$ with the equations given below derived here to implement the constraints of the embedding function.

parameter	***value***
$f_e / 10^{-18}$ C nm^{-3}	0.56638674
β	5.75486
$Z_e / 10^{-18}$ C	0.021945331
α	4.2369
$F(\rho_e)$ / eV	-1.73505924326
$F'(\rho_e)$ / eV nm^3 C^{-1}	$-2.248592 \cdot 10^{17}$
$F''(\rho_e)$ / eV nm^6 C^{-2}	$5.0047652 \cdot 10^{31}$
F_{b3} / eV nm^9 C^{-3}	$1.3050788 \cdot 10^{51}$
r_e / nm	0.2665
$\rho_e / 10^{-18}$ C nm^{-3}	5.7382624
$\rho_{max} / 10^{-18}$ C nm^{-3}	21.083445

$$F_{a0} = \frac{F(\rho_e)}{\rho_e} \qquad F_{a1} = \frac{F'(\rho_e)\rho_e - F(\rho_e)}{\rho_e^2} \qquad F_{a2} = \frac{F''(\rho_e)\rho_e^2 - 2F'(\rho_e)\rho_e + 2F(\rho_e)}{3\rho_e^2}$$

$$F_{b0} = F(\rho_e) \qquad F_{b1} = F'(\rho_e) \qquad F_{b2} = 0.5\ F''(\rho_e)$$

Electronic supplementary material Table 2: CNA signatures for the hcp structure. The letters A and B indicate to which layer of the plane the atom belongs, in case the surface consists of two planes. Existing structures with the same signature are listed too.

Structure	***#nn***	***CNA(#),…***
Bulk	12	422(6), 421(6)
(0001) A/B- layer ≡ *fcc* (111) *plane*	9	421(3), 311(6)
$(10\bar{1}0)$ A-layer ≡ *icosa. surface edge*	8	422(2), 322(2), 311(4)
$(10\bar{1}0)$ B- layer ≡ *deca. bulk*	10	422(2), 421(2), 311(4), 300(2)
$(1\bar{1}00)$ A- layer	6	422(2), 211(2), 100(2)
$(1\bar{1}00)$ B- layer	10	422(2), 421(4), 322(2), 211(2)
$(10\bar{1}1)$ A- layer ≡ $(1\bar{1}01)$ B ≡ $(1\bar{1}02)$ B	9	422(2), 421(2), 322(2), 311(2), 211(1)
$(1\bar{1}01)$ A- layer ≡ $(10\bar{1}1)$ B ≡ $(10\bar{1}2)$ B	8	422(2), 421(1), 311(2), 211(1), 200(2)
$(10\bar{1}2)$ A- layer ≡ *fcc* (111)-(100) *edge*	7	421(2), 311(2), 211(3)
$(1\bar{1}02)$ A- layer ≡ *fcc* (111)-(111) *edge*	7	421(1), 311(4), 200(2)
$(11\bar{2}0)$ A/B- layer ≡ *deca. notch vertex*	7	422(1), 322(1), 311(2), 300(1), 200(2)
$(11\bar{2}1)$ A/B- layer	7	422(1), 421(1), 322(1), 311(1), 211(2), 200(1)
$(11\bar{2}\frac{1}{2})$ A- layer	6	422(1), 322(1), 311(1), 211(1), 200(2)
(0001)-$(10\bar{1}0)$-edge ≡ *tetra. edge*	6	311(4), 211(2)
(0001)-$(1\bar{1}00)$-edge	5	311(2), 211(1), 100(2)
(0001)-$(10\bar{1}0)$-$(1\bar{1}00)$-vertex ≡ *octa.*	6	421(1), 311(2), 211(2), 200(1)