

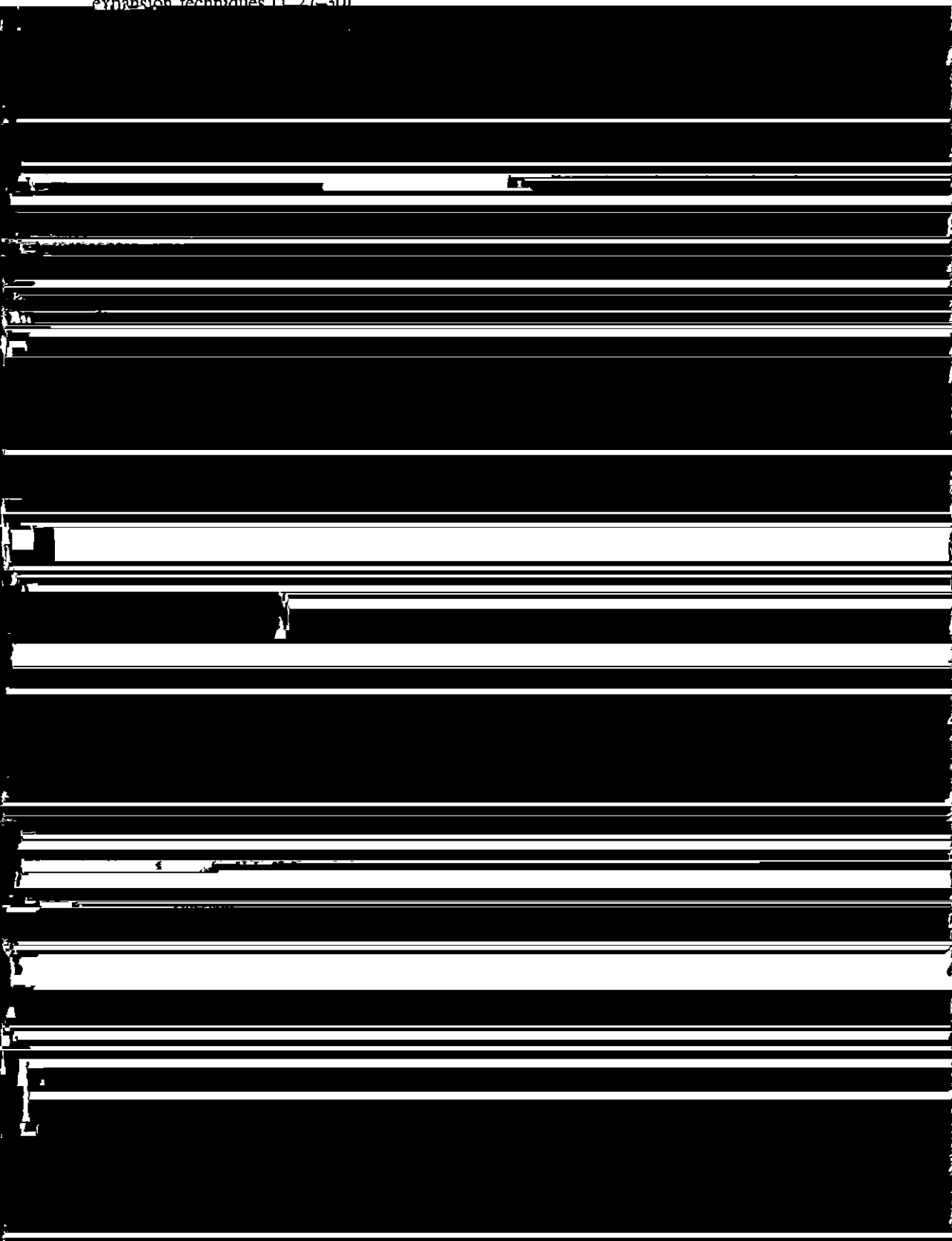
the Ag-Au system

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atom, and (2) a set of interaction energies $\{I_{ij}\}$ among the various sites belonging to a

expansion techniques [1, 27-30]



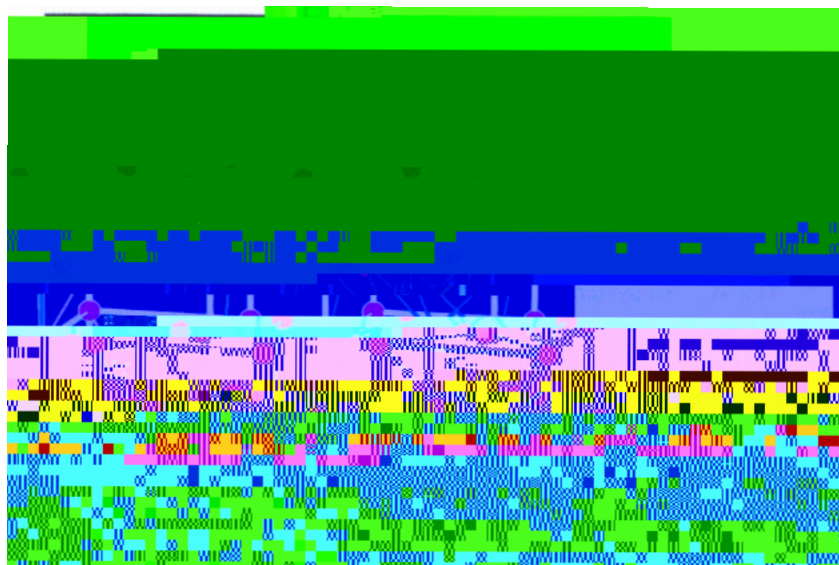


Figure 1. Geometric figures used in our cluster expansion. The expansion includes pair figures, three-body figures, and four-body figures. See table 3 for the definition of the figure coordinates.

many-body terms). We determine the N_J interaction parameters $\{J_F\}$ by mapping N_σ directly calculated $\Delta E_{\text{direct}}(\sigma)$ values onto $\Delta E_{\text{CE}}(\sigma)$ of equation (3) through a least-squares fitting procedure, i.e. by minimizing

$$\sum_{\sigma_s}^{N_\sigma} |\Delta E_{\text{direct}}(\sigma_s) - \Delta E_{\text{CE}}(\sigma_s)|^2 = \text{min} \quad (4)$$

simultaneously. Convergence is tested by applying equation (3) to a set of Γ structures (σ_i), not used in constructing the cluster expansion for equation (4). We define the quality

of the fit as $Q = \sum_{\sigma_i} |\Delta E_{\text{direct}}(\sigma_i) - \Delta E_{\text{CE}}(\sigma_i)|^2$. We use Q to compare the quality of the fit for different values of N_J and N_σ .

For the present study, we use the LDA-based non-orthogonal linearized augmented plane wave (NLAPW) method [58] to calculate the total energy of the Γ structures. We use the LDA-based NLAPW method to calculate the total energy of the Γ structures. We use the LDA-based NLAPW method to calculate the total energy of the Γ structures.

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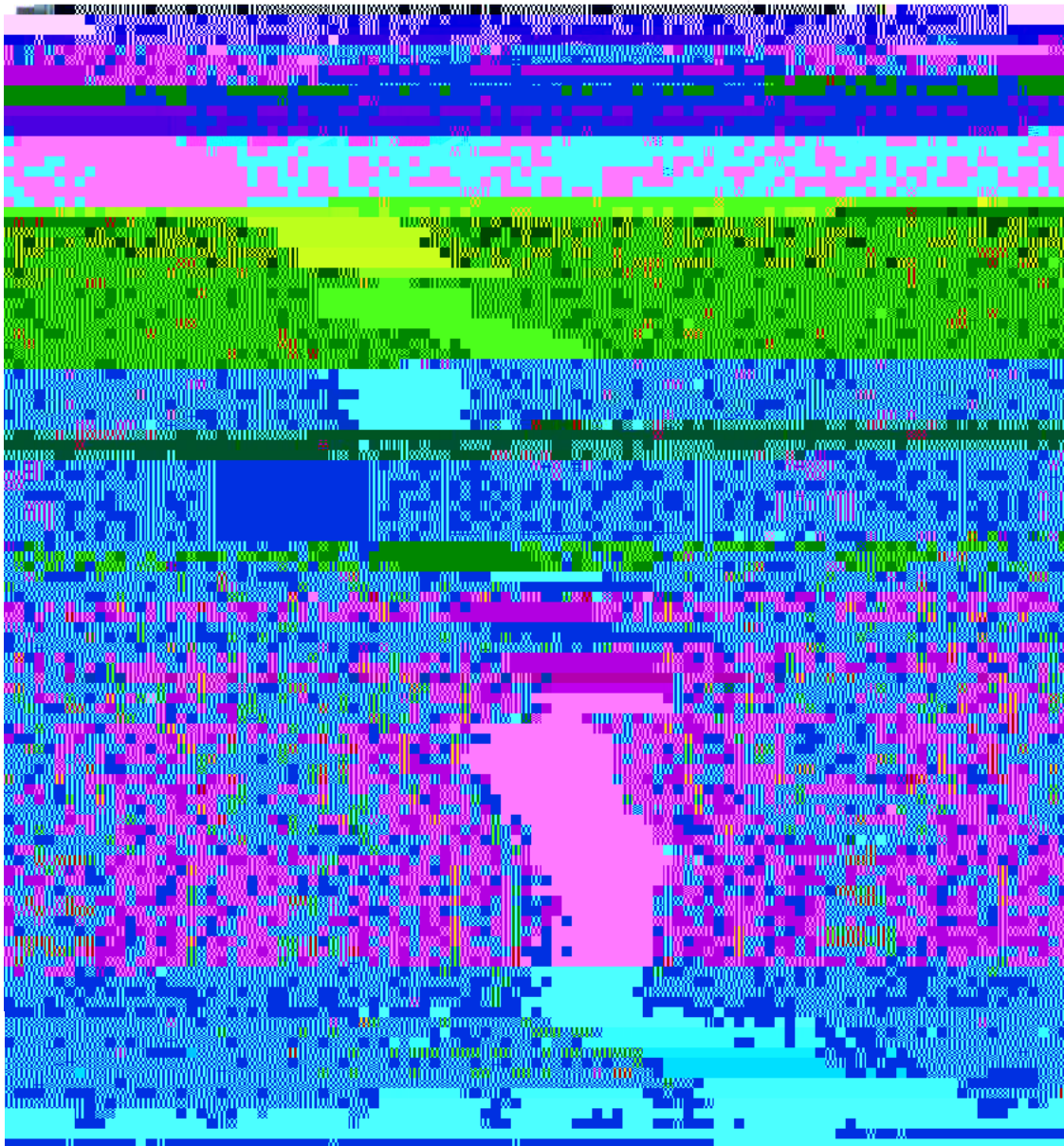
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examples of non-simply hexagonal ordered structures discussed in the introduction. Table 1 shows the unit cell parameters for these structures. The structures can be described as $A_m B_n$ superlattices along some orientation as shown in figure 2 and table 1. The structures are calculated using the same method as the simple hexagonal structure by ~ 15 meV/atom). To obtain more precise results we use a k -point sampling scheme that is geometrically equivalent to the simple hexagonal structure.

Table 1. The directly calculated LAPW excess energies $\Delta E_{\text{direct}}(\sigma)$ (error $\sim \pm 2$ meV/atom) (equation (2)), the cluster-expanded energy $\Delta E_{\text{CE}}(\sigma)$ (equation (3)), and the prediction error

Table 2. This table illustrates the effects of k -point sampling on the calculated ΔE_{direct} (in meV/atom) of some ordered compounds. The structures are defined in table 1. We have

Table 1. Characteristics of the 100 patients with primary biliary cirrhosis

Characteristic	Number (%)
Age at diagnosis (years)	61.2 (range 45-85)
Female:male	92:8
Duration of disease (years)	12.5 (range 1-35)
Time to diagnosis (years)	10.8 (range 1-30)
Time to liver transplantation (years)	11.5 (range 1-30)

liver transplantation. The mean age at diagnosis was 61.2 years (range 45-85 years) and the mean duration of disease was 12.5 years (range 1-35 years). The mean time to diagnosis was 10.8 years (range 1-30 years) and the mean time to liver transplantation was 11.5 years (range 1-30 years).

The clinical features of the 100 patients are summarized in Table 1. The most common symptoms were fatigue (95%), weight loss (85%), pruritus (80%), and jaundice (75%). The most common signs were xanthopsia (80%), scleritis (75%), and arthralgia (70%).

The laboratory findings are summarized in Table 2. The most common abnormalities were elevated alkaline phosphatase (95%), elevated gamma-glutamyl transaminase (85%), and elevated bilirubin (75%). The most common serological findings were positive antimitochondrial antibody (95%), positive antinuclear antibody (85%), and positive smooth muscle antibody (75%).

The histological findings are summarized in Table 3. The most common findings were portal inflammation (95%), bile duct damage (85%), and bile duct loss (75%). The most common histological patterns were non-preserved architecture (95%), bridging fibrosis (85%), and cirrhosis (75%).

The clinical course of the 100 patients is summarized in Table 4. The most common complications were liver failure (95%), portal hypertension (85%), and hepatocellular carcinoma (75%). The most common causes of death were liver failure (95%), portal hypertension (85%), and hepatocellular carcinoma (75%).

The survival of the 100 patients is summarized in Table 5. The median survival was 11.5 years (range 1-30 years). The most common causes of death were liver failure (95%), portal hypertension (85%), and hepatocellular carcinoma (75%).

The quality of life of the 100 patients is summarized in Table 6. The most common problems were fatigue (95%), weight loss (85%), pruritus (80%), and jaundice (75%). The most common quality of life scores were low (95%), poor (85%), and very poor (75%).

The cost of the 100 patients is summarized in Table 7. The most common costs were liver transplantation (95%), medical care (85%), and hospitalization (75%). The most common cost categories were liver transplantation (95%), medical care (85%), and hospitalization (75%).

The impact of the 100 patients is summarized in Table 8. The most common impacts were liver transplantation (95%), medical care (85%), and hospitalization (75%). The most common impact categories were liver transplantation (95%), medical care (85%), and hospitalization (75%).

The prognosis of the 100 patients is summarized in Table 9. The most common prognoses were liver failure (95%), portal hypertension (85%), and hepatocellular carcinoma (75%). The most common prognosis categories were liver failure (95%), portal hypertension (85%), and hepatocellular carcinoma (75%).

The treatment of the 100 patients is summarized in Table 10. The most common treatments were liver transplantation (95%), medical care (85%), and hospitalization (75%). The most common treatment categories were liver transplantation (95%), medical care (85%), and hospitalization (75%).

The follow-up of the 100 patients is summarized in Table 11. The most common follow-up findings were liver failure (95%), portal hypertension (85%), and hepatocellular carcinoma (75%). The most common follow-up categories were liver failure (95%), portal hypertension (85%), and hepatocellular carcinoma (75%).

The management of the 100 patients is summarized in Table 12. The most common management strategies were liver transplantation (95%), medical care (85%), and hospitalization (75%). The most common management categories were liver transplantation (95%), medical care (85%), and hospitalization (75%).

The outcomes of the 100 patients is summarized in Table 13. The most common outcomes were liver failure (95%), portal hypertension (85%), and hepatocellular carcinoma (75%). The most common outcome categories were liver failure (95%), portal hypertension (85%), and hepatocellular carcinoma (75%).

The conclusions of the 100 patients is summarized in Table 14. The most common conclusions were liver failure (95%), portal hypertension (85%), and hepatocellular carcinoma (75%). The most common conclusion categories were liver failure (95%), portal hypertension (85%), and hepatocellular carcinoma (75%).

The implications of the 100 patients is summarized in Table 15. The most common implications were liver failure (95%), portal hypertension (85%), and hepatocellular carcinoma (75%). The most common implication categories were liver failure (95%), portal hypertension (85%), and hepatocellular carcinoma (75%).

(AB). Using this original Connolly-Williams procedure, we obtained an average prediction error of $\delta_{PE} = 1.6$ meV/atom and a maximum prediction error of 4.4 meV/atom for 27 other structures that are not used in obtaining the interaction J values. The prediction errors for some specific structures are unsatisfactory. For example δ_{PE} are 4.4, 2.4, 3.0, 2.6 meV/atom, for structures '40', $\gamma 2$, DO_{22} ($AgAu_3$), and W3, respectively (larger than the estimated error of direct LDA calculation of 2 meV/atom). The large error for '40' and DO_{22} is because the Connolly-Williams set of interactions creates a spurious degeneracy

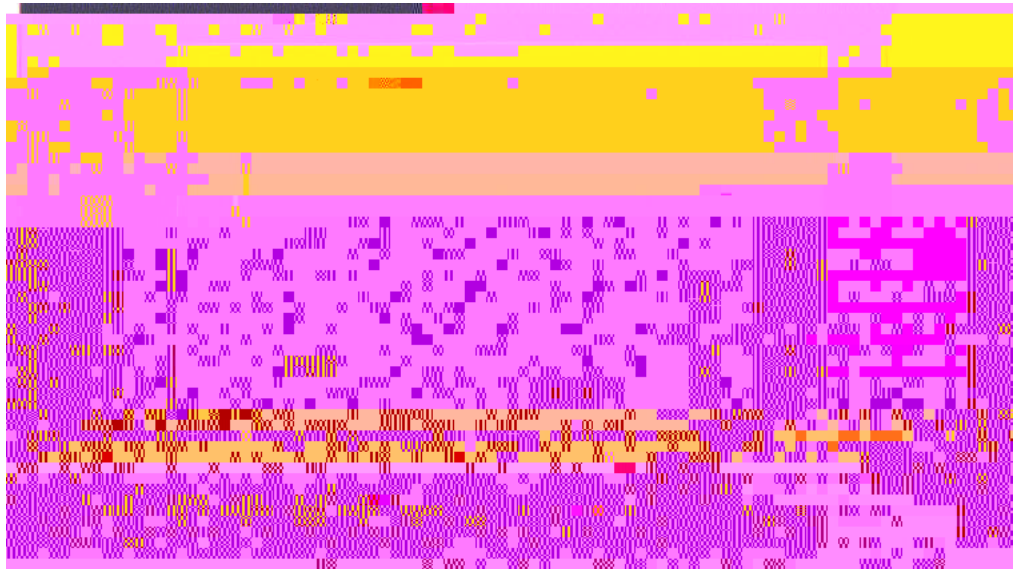


Figure 3. This figure illustrates the interaction energies (including the degeneracy $D(F, F)$) used in this work (figure 1) for fit I (table 3). The interaction energies for fit II are nearly indistinguishable on this scale. Note that the nearest-neighbor pair interaction J_1 is dominant.

that S is our definition of the 'figures' F used in our cluster expansion in terms of the

$$\frac{1}{N} \sum_{i=1}^N \mathbf{V}_i$$

$$\frac{1}{N} \sum_{i=1}^N \mathbf{V}_i^2$$

Cluster type: D (diamond), S (square), V (triangle)

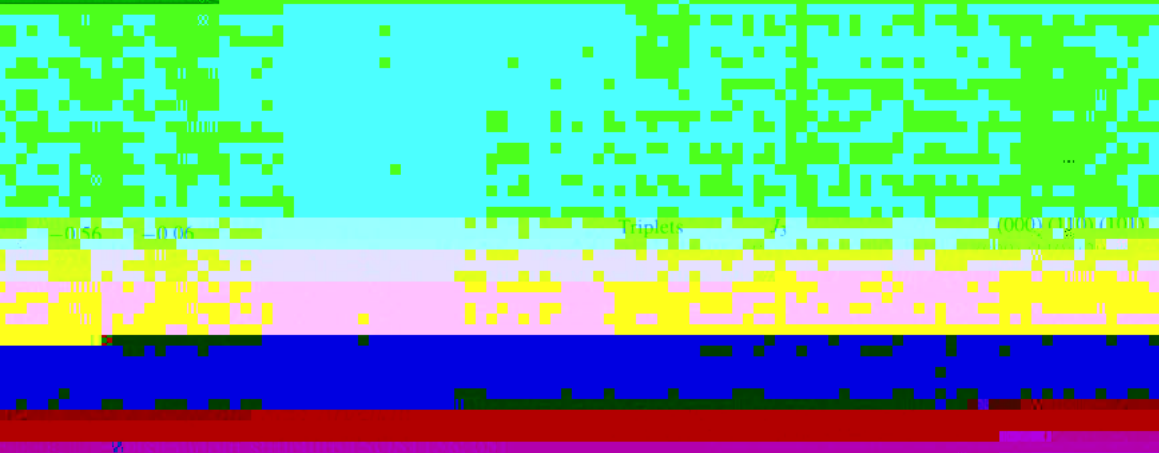


Figure 4. Density of states of random clusters.

previously to that of the density of states of random

clusters, which is

$$\rho(\mathbf{V}) = \sum_{i=1}^N \delta(\mathbf{V} - \mathbf{V}_i) \quad (10)$$

where δ is the Dirac delta function.

Figure 4 shows the density of states of random clusters (10) for the

clusters



Figure 4. Calculated and measured mixing energy for Ag-Au. The $T = 800$ K. (Jozengs) are cited from [23]. We give the calculated values

Table 4. The experimental [23] and calculated (fit δ) $\Delta H(x, T)$ mixing enthalpy $H(x, T)$

order	$\Delta H(x, T) = 800$ K		$\Delta H(x, T \rightarrow \infty)$	
	Exp [23]	Monte Carlo simulation $T = 800$ K	Monte Carlo $T = 800$ K	Calc. (equation (6)) $T \rightarrow \infty$
0.0	0.0	0.0	0.3	0.3

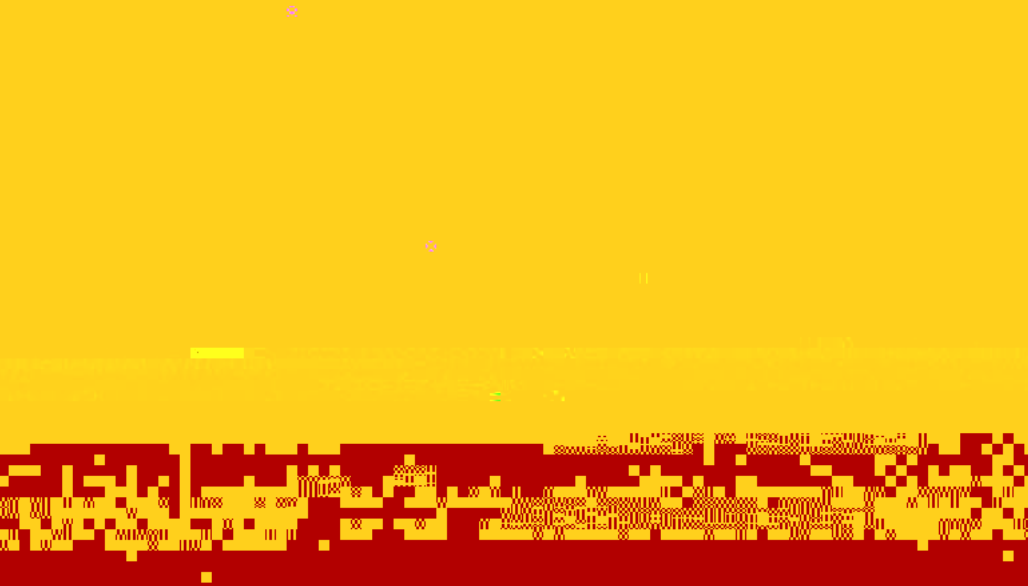


Table 5. The order-disorder phase transition temperatures T_c for $\text{Ag}_{1-x}\text{Au}_x$ alloys at $x = \frac{1}{4}$, $\frac{1}{2}$, and $\frac{3}{4}$. The calculated results were obtained using N_J interactions, solving the ensuing Ising model with the Monte Carlo (MC) method or with the cluster variation method (CVM). The 'measured' data were obtained by (i) using an inverse Monte Carlo method to extract three composition-dependent effective pair interactions from the short-range order data of the Georgopoulos-Cohen (GC) and Borier-Sparks (BS) analyses and (ii) subjecting the these effective interactions to a direct Monte Carlo simulation.

		Ag ₃ Au <i>L</i> ₁₂	AgAu <i>L</i> ₁₀	AgAu ₃ <i>L</i> ₁₂
Calculated (K)				
Present, fit I	$N_J = 12$; MC	155	210	225
Wei <i>et al</i> ^a	$N_J = 5$; CVM	120	240	200
Mohri <i>et al</i> ^b	$N_J = 5$; CVM	152	177	183
'Measured' (K)				
Schönfeld <i>et al</i> (BS) ^c	$N_J = 3$; MC	115	115	155
Schönfeld <i>et al</i> (GC) ^d	$N_J = 3$; MC	165	165	210
Norman and Warren ^e		90		
Ziesemer ^f			168	





Figure 6. Calculated (a) and experimental (b) [15] diffuse-scattering intensities due to short-range order in α -Fe₃C. The calculation was done at $T = 600$ K, while the experiment was performed on a sample that was homogenized at $T = 1173$ K and later aged at $T = 515$ K.

values with experiment [23]. The agreement is excellent. Note that the finite-temperature enthalpy $H(T)$ is calculated at $T = 600$ K, which is not the same as the experimental temperature. The agreement between the calculated $H(T)$ and the experimental $H(T)$ is excellent, and by Ackland and Vitek [25] and the semiempirical method by Brozillo and coworkers [26].

The ground state problem can be solved by using the linear programming method in T_0 or by allowing the system to relax completely. Searches for the ground state were given over Kan and coworkers [27] and by Ackland and Vitek [25] and the semiempirical method by Brozillo and coworkers [26].

3.4. $T = 0$ ground state structures

The ground state problem can be solved by using the linear programming method in T_0 or by allowing the system to relax completely. Searches for the ground state were given over Kan

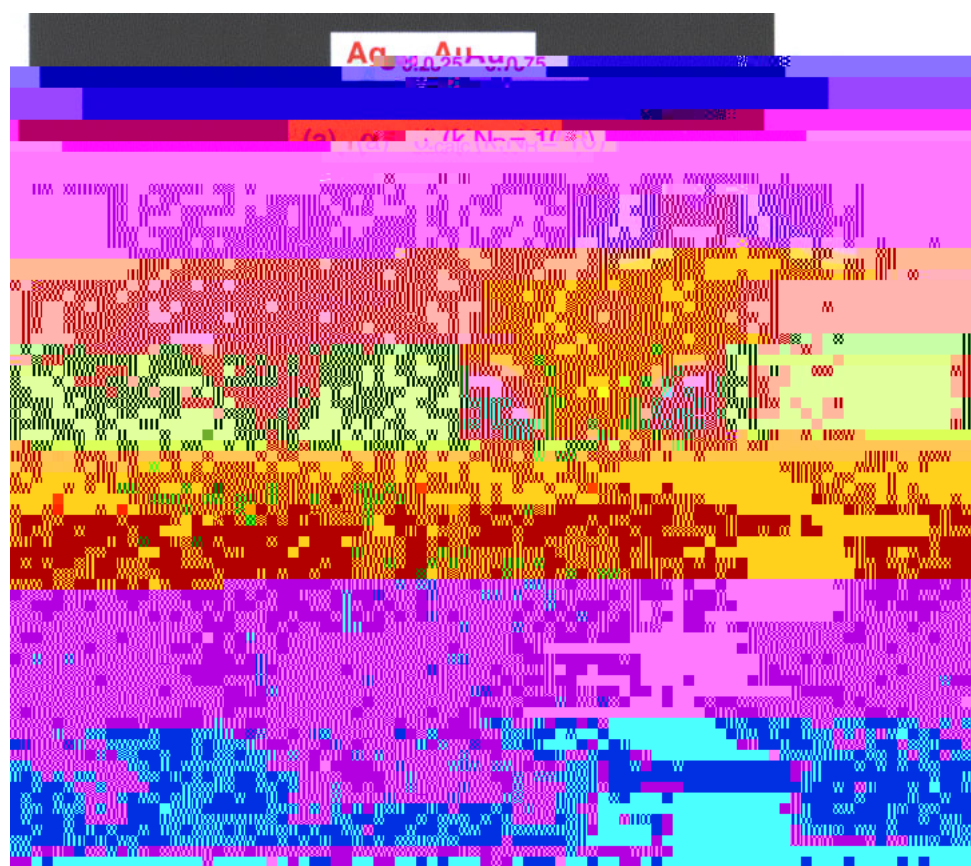
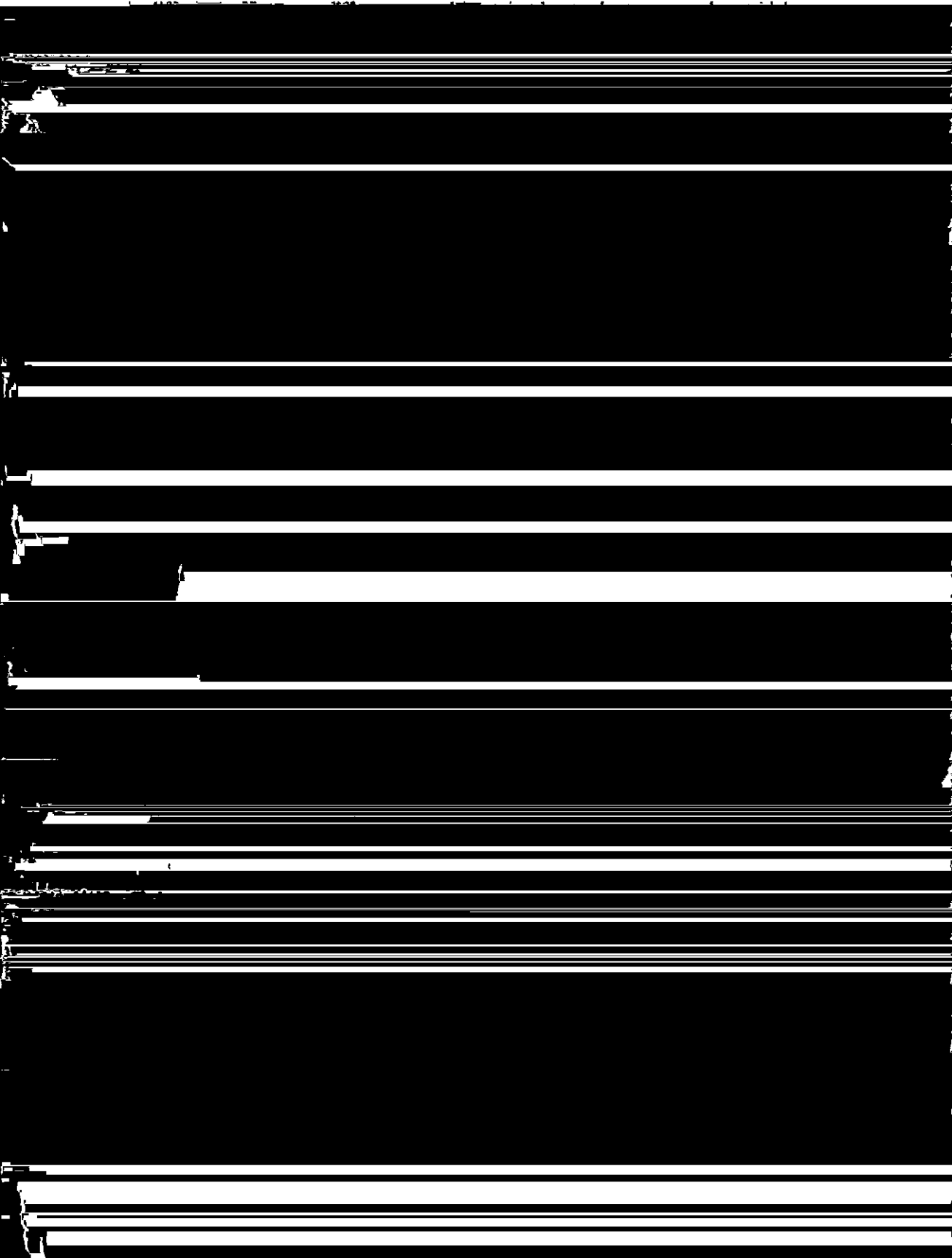


Figure 7. Calculated (a) and experimental (b) [110] diffuse-scattering intensity profiles for $\text{Ag}_{0.75}\text{Au}_{0.25}$, which were Fourier synthesized using $N_{\text{range_order}} = 10$ real coordinates $\delta(\mathbf{k}_{\text{min}})$ (including $\sigma(P_{\text{min}}) = 1$ for both experiment and theory). The calculation was done at $T = 600$ K, the same as the experiment.

structure is described in terms of its lattice averaged products Π_F which do not always correspond to a physical arrangement of atoms in the structure. Here, we will use the Monte Carlo simulated annealing algorithm to perform a



difference at $x = 0.5$ is -4.4 meV/atom, correlating with a fairly pronounced peak at the X point for $\alpha_{\text{SRO}}(\mathbf{k})$ at $x = 0.523$.

4. Conclusions

We have demonstrated here that accurate alloy properties can be obtained from *ab initio* calculated total energies for 20 simple structure and body centered cubic (bcc) structures.

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