Section I. Derivation of the Mean-Field NP Probability Distribution

In this section we show how to obtain Eq. 5 in the main text. We pick up the derivation from the main text starting with \( P(\gamma) = \frac{Q'}{Q} \exp \left[ -\beta U_m(\gamma) \right] \). Plugging \( Q' = CQ (N - 1, N, \int [V(w) - \nu_p(w, \gamma)] d\vec{w}, T) \) into \( P(\gamma) \) and taking the natural logarithm of both sides gives,

\[
\ln[P(\gamma)] = -\beta U_m(\gamma) + \ln \left[ Q \left( N - n_r, N, \int [V(w) - \nu_{p,n_r}(w, \gamma)] d\vec{w}, T \right) \right] - \ln [Q(N, N, V, T)] \quad (I.1)
\]

Here, we use a generalized form for \( Q' \) (employing \( n_r \) instead of 1) to facilitate taking the multidimensional Taylor expansions of \( \ln(Q) \) and \( \ln(Q') \) about \( n_r = 0 \) and \( \nu_{p,0} = \nu_p \). Truncating terms of second or higher order yields

\[
\ln[P(\gamma)] = -\beta U_m(\gamma) - \int \frac{\partial \ln [Q(N, N, V, T)]}{\partial \nu_p(\gamma, w)} \nu_p(\gamma, w) d\vec{w} - \frac{\partial \ln [Q(N, N, V, T)]}{\partial n_r} n_r(\gamma, w) \quad (I.2)
\]

We now recognize that \( -\beta \mu_p(\gamma) = \partial \ln (Q) / \partial n_r \) and \( \beta \pi(\gamma, w) = \partial \ln Q / \partial \nu_p(\gamma, w) \), where \( \mu_p(\gamma) \) is the particle chemical potential and \( \pi(\gamma, w) \) is a pressure term for the \( w \)th volume element. Substituting gives the desired probability distribution function (pdf) of interest for a reference particle with configuration \( \gamma \) within the system

\[
P(\gamma) = \exp \left[ -\beta \left( U_m(\gamma) + \int \pi(\gamma, w) \nu_p(\gamma, w) d\vec{w} - \mu_p(\gamma) n_r(\gamma) \right) \right] \quad (I.3)
\]

This last expression is identical to Eq. 5 in the main text (for \( n_r = 1 \)).
Section II. Obtaining Eq. 5 in the Main Text from a Lattice Model

It is worthwhile to comment on the functional form for $P(\gamma)$. Suppose we perform a discretization into $M$ layers for a lattice commensurate with anisotropic particle geometry (i.e. triangular lattice for triangles, square lattice for squares, or hexagonal lattice for hexagons). An analogous set of equations can be written without the need of pseudoparticles because the lattice site positions are discrete. In this limit, there is no void space within the system to fit pseudoparticles. This constraint takes the form of

$$\langle \rho_m(\gamma) \rangle = \sum_{\gamma} P(\gamma) \rho_m(\gamma) \quad (\text{II.1})$$

where $\rho_m$ is the volume fraction in the $m$th layer given particle configuration $\gamma$. We write the entropy as

$$S = -k \sum_s P(\gamma) \ln[P(\gamma)]$$

where subscript $s$ indicates a summation over all possible microstates. Maximization of entropy subjected to the $M-1$ layer constraints defined in Eq. II.1 follows standard procedures $[?]$ and gives

$$P(\gamma) = Q^{-1} \exp \left[ -\sum_{m=1}^{M-1} \lambda_m \rho_m(\gamma) \right] \quad (\text{II.2})$$

where $Q = \sum_{\gamma} \exp \left[ \sum_{m=1}^{M-1} \lambda_m \rho_m(\gamma) \right]$ is the partition function and $\lambda_m$ in Eq. II.2 is the Lagrange multiplier corresponding to the $m$th layer from constraints in Eq. II.1. $\lambda_m$ is defined via

$$\lambda_m = \frac{\partial \ln Q}{\partial \rho_m} \quad (\text{II.3})$$

Just as $P$ and $V$ are conjugate thermodynamic variables, $\lambda_m$ is a pressure term that is the conjugate of the particle volume. We now compare Eq. I.3 with Eq. II.2. In the limit of no pseudoparticles, $U_m = 0$ and $\mu_p = 0$ for Eq. I.3. Taking the same limits for Eq. I.3 reduces it to

$$P(\gamma) \sim \exp \left[ -\beta \left( \int \pi(\gamma, w) \nu_p(\gamma, w) \, dw \right) \right] \quad (\text{II.4})$$

By inspection, Eq. II.4 is the continuous limit of Eq. II.2. The resulting mean-field approximation for $P(\gamma)$ as defined by Eq. I.3 is therefore the pdf that maximizes the total entropy of the system. As a result, subsequent application of the pdf in Eq. I.3 for determining colloidal crystal structure with the lowest relative total energy can be interpreted as selecting for the crystal structure that maximizes entropy.
Section III. Deriving Eq. 7 from Eqs. 5 and 6 in the Main Text

To develop a functional form for the pP-NP interaction potential \( U_m \), we take Eq. I.3 and rearrange for \( U_m \) to obtain the desired mean-field interaction potential of interest between particles and pseudoparticles.

\[
\beta U_m = \beta \mu_p (\gamma) n_r (\gamma, w) - \ln [P (\gamma, w)] - \beta \pi (\gamma, w) \nu_p (\gamma, w) \quad \text{(III.1)}
\]

We can then solve for \( \pi (\gamma, w) \) in Eq. 6 from the main text and plug the result into Eq. III.1 to give

\[
\beta U_m = \beta \mu_p (\gamma) n_r (\gamma, w) - \ln [P (\gamma, w)] - \nu_p (\gamma, w) \nu_p^{-1} (w) \left[ \beta \mu_{pP} (\gamma) - \ln [\rho_{pP} (\gamma, w)] \right] \quad \text{(III.2)}
\]

\[
\beta U_m = \left[ \frac{\nu_p (\gamma, w)}{\nu_p (\gamma, w)} \right] \left[ \frac{\nu_p (w)}{\nu_p (\gamma, w)} \right] \left[ \beta \mu_p (\gamma) n_r (\gamma, w) - \ln [P (\gamma, w)] - \beta \mu_{pP} (\gamma) + \ln [\rho_{pP} (\gamma, w)] \right] \quad \text{(III.3)}
\]

In the limit of \( \nu_{pP} \ll \nu_p \), Eq. III.3 simplifies to

\[
\beta U_m (w) = \left[ \frac{\nu_p (\gamma, w)}{\nu_p (\gamma, w)} \right] \left[ \ln [\rho_{pP} (\gamma, w)] - \beta \mu_{pP} (\gamma) \right] \quad \text{(III.4)}
\]

As we move radially away from the reference particle (i.e as \( w \) increases), we expect that the ratio of volume contribution between particles and pseudoparticles \( \nu_p / \nu_{pP} \) to decrease with the differential volume element \( dV \sim w^2 dw \). Plugging in this approximation gives Eq. 7 in the main text.

\[
\beta U_m (w) = \frac{1}{w^2} \left[ \ln [\rho_{pP} (\gamma, w)] - \beta \mu_{pP} (\gamma) \right] + \sum_i^N U_{core} (\gamma, w) \quad \text{(III.5)}
\]

where we added back in the hard core repulsion \( (U_{core}) \) preventing pseudoparticles from sitting inside a nanoparticle implicit in the various \( (') \) of our configurational integrals.
Section IV. Derivation of Shape Orbitals

Here we analytically derive the series of shape harmonics used in the manuscript that explicitly accounts for polyhedron geometry in the solution of the eigenvalue equation (Eq. 9 in main text), thereby reducing the complexity of the trial basis function. We start with the general form of the Laplacian in an arbitrary coordinate system:

\[
\nabla^2 = \frac{1}{h_u h_v h_w} \left[ \frac{\partial}{\partial u} \left( \frac{h_v h_w}{h_u} \frac{\partial}{\partial u} \right) + \frac{\partial}{\partial v} \left( \frac{h_u h_w}{h_v} \frac{\partial}{\partial v} \right) + \frac{\partial}{\partial w} \left( \frac{h_u h_v}{h_w} \frac{\partial}{\partial w} \right) \right] \tag{IV.1}
\]

\[
h_u = \left[ \left( \frac{\partial x}{\partial u} \right)^2 + \left( \frac{\partial y}{\partial u} \right)^2 + \left( \frac{\partial z}{\partial u} \right)^2 \right]^{1/2} \tag{IV.2}
\]

\[
h_v = \left[ \left( \frac{\partial x}{\partial v} \right)^2 + \left( \frac{\partial y}{\partial v} \right)^2 + \left( \frac{\partial z}{\partial v} \right)^2 \right]^{1/2} \tag{IV.3}
\]

\[
h_w = \left[ \left( \frac{\partial x}{\partial w} \right)^2 + \left( \frac{\partial y}{\partial w} \right)^2 + \left( \frac{\partial z}{\partial w} \right)^2 \right]^{1/2} \tag{IV.4}
\]

where \( u, v, \) and \( w \) are generalized coordinates, converted from \( x, y, \) and \( z \) using a set of parametric equations. In general, the parameterizations are: \( x(u,v,w) = f_1(u,v,w), y(u,v,w) = f_2(u,v,w), z(u,v,w) = f_3(u,v,w). \) Our first approximation is to define a set of parameterizations where \( w \) (taken to be the radial component) is a multiplicative prefactor to a convolution of the two angular components \((u,v).\) As a clarifying example, for an octahedron we can write

\[
x(u,v,w) = wc(v,2)c(u,2) \tag{IV.5}
\]

\[
y(u,v,w) = wc(v,2)s(u,2)
\]

\[
z(u,v,w) = ws(v,2)
\]

where \( s(a,b) = \text{sgn}[\sin(a)] |\sin(a)|^b \) and \( c(a,b) = \text{sgn}[\cos(a)] |\cos(a)|^b, \) with \( \text{sgn}[f(x)] \) defined as the sign function for \( f(x) \). Plugging Eq. IV.5 into Eq. IV.2 - IV.4 gives

\[
h_u^2 = 8w^2 [\cos^4(v)] [\cos^2(u) \sin^2(u)] \tag{IV.6}
\]

\[
h_v^2 = 4w^2 [\cos^2(v) \sin^2(v)] [\cos^4(u) + \sin^4(u) + 1] \tag{IV.7}
\]
\[ h_w^2 = \cos^4(v) \left[ \cos^4(u) + \sin^4(u) \right] + \sin^4(v) \]  

(IV.8)

This parameterization reduces the geometry of the coordinate system to that of contours emanating from an origin that conforms to the surface of the shape (here, polyhedra) of interest. These contours are first set by spherical rings at distances \( w \) away from the origin, that are then morphed into the correct shape by a shape kernel, \( \Omega \), that is only a function of the angular component. \( \Omega \) is now taken to be a pre-averaged value and is approximated to be a constant upon expanding in \( \partial / \partial u \) and \( \partial / \partial v \). In terms of our pseudoparticle cloud, this approximation implies that pseudoparticles reorganize on a much faster timescale than the rotational relaxation of the polyhedra. The functional form of \( h_w \) satisfies the requirements for our shape kernel and thus we define \( \Omega(u, w) = h_w(u, w) \). Our second approximation involves defining an in-plane (here, xy plane) kernel, \( \Gamma \), analogous to the overall shape kernel that is only a function of either \( u \) or \( v \). By inspection, \( \Gamma_u = \cos^4(u) + \sin^4(u) \) satisfies this requirement. Substituting the above definition into Eqs. IV.6 - IV.8 gives

\[ h_u^2 = 4w^2 \Gamma_v^2 (1 - \Gamma_u) \]  

(IV.9)

\[ h_v^2 = 4w^2 \Gamma_v (1 - \Gamma_v) (1 + \Gamma_u) \]  

(IV.10)

\[ h_w^2 = \Omega^2 \]  

(IV.11)

where we introduced \( \Gamma_v = \cos^2(v) \). Plugging Eqs. IV.9 - IV.11 into the relevant terms in Eq. IV.1 gives

\[ [h_u h_v h_w]^{-1} = \left\{ \left[ 16w^4 \Omega^2 \Gamma_v^3 (1 - \Gamma_v) (1 - \Gamma_u^2) \right]^{1/2} \right\}^{-1} = [4w^2 \Omega A_u A_v]^{-1} \]  

(IV.12)

\[ \frac{h_u h_w}{h_u} = \left\{ \Omega^2 \left[ \frac{1 + \Gamma_u}{1 - \Gamma_u} \right] \left[ \frac{1 - \Gamma_v}{\Gamma_v} \right] \right\}^{1/2} = \Omega B_u B_v \]  

(IV.13)

\[ \frac{h_u h_w}{h_v} = \left\{ \Omega^2 \left[ \frac{1 - \Gamma_u}{1 + \Gamma_u} \right] \left[ \frac{\Gamma_v}{1 - \Gamma_v} \right] \right\}^{1/2} = \Omega C_u C_v \]  

(IV.14)

\[ \frac{h_u h_w}{h_w} = \left\{ \left[ \frac{16w^4}{\Omega^2} \right] \left[ 1 - \Gamma_u^2 \right] \left[ \Gamma_v^3 (1 - \Gamma_v) \right] \right\}^{1/2} = \left( \frac{4w^2}{\Omega} D_u D_v \right) \]  

(IV.15)

where \( A_u, B_u, C_u, \) and \( D_u \) group the purely \( u \)-dependent terms in Eqs. IV.12 - IV.15. Similarly, \( A_v, B_v, \)
$C_v$ and $D_v$ group the purely $v$-dependent terms. Plugging Eqs. IV.12 - IV.15 into the original Laplacian (Eq. IV.1) gives

$$\nabla^2 = \frac{1}{4w^2\Omega^2} \left\{ \left( \frac{\Omega^2}{A_u A_v} \right) \left[ \frac{\partial}{\partial u} \left( B_u B_v \frac{\partial}{\partial u} \right) + \frac{\partial}{\partial v} \left( C_u C_v \frac{\partial}{\partial v} \right) \right] + \frac{\partial}{\partial w} \left( w^2 \frac{\partial}{\partial w} \right) \right\} \quad \text{(IV.16)}$$

This allows us to define a separation of variables $\nabla^2 \Phi(u, v, w) = \nabla^2 [S(w) T(u, w)]$ to give

$$\frac{1}{S_w} \frac{\partial}{\partial w} \left[ w^2 \frac{\partial S_w}{\partial w} \right] = K \quad \text{(IV.17)}$$

$$\left( \frac{1}{T_{uv}} \right) \left( \frac{\Omega^2}{A_u A_v} \right) \left[ \frac{\partial}{\partial u} \left( B_u B_v \frac{\partial T_{uv}}{\partial u} \right) + \frac{\partial}{\partial v} \left( C_u C_v \frac{\partial T_{uv}}{\partial v} \right) \right] = -K \quad \text{(IV.18)}$$

where $S_w = S(w)$, $T_{uv} = T(u, v)$ and $K$ is a constant to be solved for. Simplifying Eq. IV.18,

$$\left( \frac{\Omega^2}{T_{uv}} \right) \left[ \frac{B_v}{A_v} \frac{1}{A_u} \frac{\partial}{\partial u} \left( B_u \frac{\partial S_u}{\partial u} \right) + \frac{C_u}{A_u} \frac{1}{A_v} \frac{\partial}{\partial v} \left( C_v \frac{\partial S_v}{\partial v} \right) \right] = -K$$

The ratios are additionally simplified to

$$\frac{B_v}{A_v} = \left( \frac{1}{\Gamma_v} \right)^2$$

$$\frac{C_u}{A_u} = \frac{1}{1 + \Gamma_u}$$

thus giving

$$\left( \frac{\Omega^2}{T_{uv}} \right) \frac{1}{\Gamma_v^2 (1 + \Gamma_u)} \left[ \left( \frac{1 + \Gamma_u}{A_u} \right) \frac{\partial}{\partial u} \left( B_u \frac{\partial T_{uv}}{\partial u} \right) + \left( \frac{\Gamma_v^2}{\Gamma_v} \right) \frac{\partial}{\partial v} \left( C_v \frac{\partial T_{uv}}{\partial v} \right) \right] = -K \quad \text{(IV.19)}$$

Recognizing that $\Gamma^2_v (1 + \Gamma_u) = \Omega + (2\Gamma_v - 1)$ allows for a further separation of variables for $T_{uv} = S_u S_v$:

$$\left[ \left( \frac{1 + \Gamma_u}{A_u} \right) \frac{1}{S_u} \frac{\partial}{\partial u} \left( B_u \frac{\partial S_u}{\partial u} \right) \right] + \left[ \left( \frac{\Gamma_v^2}{A_v} \right) \frac{1}{S_v} \frac{\partial}{\partial v} \left( C_v \frac{\partial S_v}{\partial v} \right) + K \left( \frac{\Omega + 2\Gamma_v - 1}{\Omega^2} \right) \right] = 0 \quad \text{(IV.20)}$$

which can again be separated into

$$\left( \frac{1 + \Gamma_u}{A_u} \right) \frac{1}{S_u} \frac{\partial}{\partial u} \left( B_u \frac{\partial S_u}{\partial u} \right) = -L \quad \text{(IV.21)}$$

$$\left( \frac{\Gamma_v^2}{A_v} \right) \frac{1}{S_v} \frac{\partial}{\partial v} \left( C_v \frac{\partial S_v}{\partial v} \right) + K \left( \frac{\Omega + 2\Gamma_v - 1}{\Omega^2} \right) = L \quad \text{(IV.22)}$$
Eq. IV.17, IV.21, and IV.22 now define a series of differential equations that can all be solved via a power-series expansion in $u$, $v$, and $w$. It is straightforward though tedious to solve for these expansions and so we simply provide the final solutions (note $\rho_{pp}(u, v, w) = S(u) S(v) S(w)$):

\begin{align}
S(u) &= \sum_{j=0}^{l} a_j \left[ \Gamma_u(u) \right]^j \\
\Gamma_u(u) &= \cos^4(u) + \sin^4(u) \\
a_{j+1} &= \frac{a_j [(j + 1) (j + 1/2)] - 2a_{j-1} [j^2 - j^2]}{(j+1)(j+2)} \\
S(v) &= \sum_{j=0}^{k-1} a_j \left[ \Gamma_v(v) \right]^{2j} \\
\Gamma_v(v) &= \cos(v), \quad |k| < 2(l-1) \\
a_{j+1} &= \frac{(2\Omega)^{-1} [16l^2 - 4 \ast (k+1)^2]}{(k+1)^2 - (j+1)^2} \\
S(w) &= w^{K_{pp}} \exp \left[ -\frac{2\Omega^2 B w}{n} \right] \sum_{j=0}^{n_{m}} a_j w^j \\
a_{j+1} &= \left( \frac{4\Omega^2 B}{n} \right) \left[ \frac{j + K_{pp} + 1 - n}{(j+1)(2K_{pp} + 2 - j)} \right] \\
n_m &= 2n - \sqrt{4K_p + 1} - 1
\end{align}

with parameters

\begin{align}
K_p &= 4\Omega \left[ 4l^2 - (k+1)^2 \right] \\
K_{pp} &= \frac{1}{2} \sqrt{4K_p + 1} - \frac{1}{2}
\end{align}

Different shapes necessitate alternate functional forms for $\Omega$, which can be solved for a priori. Fig. 3a1-d1 in the main text shows the lowest order shape orbitals for four different polyhedra. The above equations for $u$, $v$ and $w$ can now be used to solve the eigenvalue equation (Eq. 9 in the main text) for the pseudoparticle density distribution $\rho_{pp}$. 

7
Section V. Hard Sphere Free Energy Calculation for FCC vs HCP

As a consistency check for known hard sphere behavior, we performed free energy calculations using entropic bond theory for the classic problem of FCC vs HCP lattice energy (Fig. V.1). Entropic bond theory reproduces the expected behavior, showing FCC is lower in free energy than HCP with a free energy difference of \( \sim 0.004 \, \text{kT} \) for \( E_{\text{HCP}} - E_{\text{FCC}} \) [1,2]. This value is congruent with results obtained by Woodcock et al. [1] but is (expectedly) higher compared to more rigorous Frenkel-Ladd type calculations [2].

Figure V.1: Entropic Bond Calculation of Lattice Free Energy of Formation for Hard Spheres arranged in an FCC vs HCP crystal structure. Expected behaviors are reproduced in our calculation, where FCC is very slightly lower in free energy than HCP by 0.004 kT.
Section VI. MD Simulations of Pseudoparticles in a Crystal of Hard Polyhedra

To further validate our use of a pseudoparticle ansatz as a mathematical device for calculating entropic bonding, we performed explicit molecular dynamics (MD) simulations of NPs and pPs. Simulations were initialized with pPs uniformly distributed throughout the system. All interactions between pPs and NPs in our systems were computed using a recently developed anisotropic potential [3] implemented in HOOMD-Blue [4, 5]. Here, we set the diameter of an individual pP to be $\sigma$. The insphere radius of the polyhedron core is $10\sigma$. The ideal (zero) interactions between pseudoparticles is approximated by a Weeks-Chandler-Anderson potential (WCA) with negligible $\epsilon = 1E - 10$. Interactions between NPs and pPs use $\epsilon = 3.0$. NPs interact via a WCA potential with $\epsilon = 1.0$, shifted to the surface of the particle. All simulations were run in the NVT ensemble at $T = 1.0kT/\epsilon$ for $1E7$ timesteps with $dt = 0.0005\sigma (m/\epsilon)^{0.5}$ in simulation units, where $m$ is mass.

![Figure V.1: Simulation validation of Shape Orbitals in Hard Polyhedra. Molecular simulation (MD) snapshots of pPs about a central NP. a) Initial configuration with pPs uniformly distributed. Subplots with subscript 1 – 4 indicate cube, tetrahedron, dodecahedron and hexagonal prism, respectively. b) pPs reorganize relative to each particle shape. Blue envelopes indicate regions of strong pP aggregation. c) Lowest order shape orbitals predicted from angular expansions of the local pP density distribution in shape space. Structures of orbitals in (c) show generally good agreement with those from MD (b).](image)

We start with simulations consisting of one polyhedron. These simulations are performed for a cube, tetrahedron, dodecahedron, and hexagonal prism. Each simulation starts with pP uniformly distributed across free space within the system (Fig. V.1a1-4). As the simulation progresses, the pPs move and develop regions of high and low pP density around the particle as the system evolves towards equilibrium. The equilibrium distribution of pPs around the particle closely resembles the lowest order shape orbitals (Fig. V.1b1-4).
clarity, we draw envelopes (light blue) about regions where pPs preferentially sit to highlight localization. Fig. V.1c-4 show that theoretical shape orbitals from harmonic expansions match well the simulation results for each shape.

Adding corrections from higher order orbitals only slightly improves the comparison of theory and simulation. Instead, the broadening of the MD results relative to the theoretical results arises from the simulated pPs having a finite diameter. Reducing the size of the pP results in extremely long computational times because of the smaller time steps needed in the simulation. However, checks of larger pP size (up to 3σ) show that the resulting pP clouds broaden even further. Thus in the limit of pPs being point particles, the MD simulations will more closely match the theoretical results.

Binary polyhedron simulations carried out using the same protocol used for simulations shown in Fig. V.1 reveal pP localization between particles that compare well with “bonding” orbitals predicted by theory, as shown in Fig. V.2 for the lowest order orbitals.

**Figure V.2: Simulation Validation of Bonding Orbitals in Hard Polyhedra.** Subplots with subscript 1–4 indicate cube, tetrahedron, dodecahedron and hexagonal prism, respectively. a) MD simulation snapshots of pP localization between polyhedra results in “bonding” orbitals between shapes. b) Theoretically predicted bonding orbitals, in good agreement with simulation results in subplots 1.

Additionally, we perform MD simulations to demonstrate pP localization for a simple cubic arrangement of cubes to visualize how the use of pPs facilitates theoretical lattice predictions. Fig. V.3a shows the theoretically predicted bonding orbitals to lowest order. Fig. V.3b shows the equilibrium MD simulation results, demonstrating localization of pPs into the interstitial spaces between cubes configured in a SC arrangement. Fig. V.3c shows MD simulation results where cubes start in a disordered fluid phase and organize into SC under the influence of pP-NP interactions. Both simulations produce bonding orbitals that match well to those predicted from theoretical calculations.
Figure V.3: Simulation Validation of Bonding Orbitals Within a Crystal. a). Theoretically predicted bonding orbitals between cubes in a SC lattice. b) MD simulation snapshot showing pPs localization about cubes to form “bonding” orbitals in the SC crystal. Visual comparison with theoretically predicted “bonding” orbitals indicate good agreement. c) MD simulation snapshot show pPs organizing freely moving/rotating cubes into the thermodynamically stable SC lattice to produce analogous “bonding” orbitals.

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