A Data Augmentation

The MEG data of Human Connectome Project (HCP) has been filtered into theta (4-8Hz),alpha (8-13Hz) and beta (13-30Hz) bands. As discussed in previous results [6, 9, 8], different filter band shows different brain connectivity. For example, the visual connectivity from visual cortex to temporal and parietal lobes is strong in alpha band. While in beta band, the connectivity through the superior parietal to occipital cortex dominates. The visual and motor connectivity is strong in theta band [7]. For fMRI data augmentation, we randomly select 1/3 of the number of voxels within each ROI to get the parcellated mean time courses as heterogeneous multiview inputs. In the framework, we utilize the filtered MEG data with alpha, beta and theta bands as heterogeneous views and learn the contrastive graph representation together with the corresponding augmented fMRI data.

B Homogeneous and Heterogeneous Modeling

The T1w/T2w map is characterized by high values in sensory regions and low values in association regions. We define the heterogeneity map using the median T1w/T2w values averaged across the whole subjects. The heterogeneity map for each node i is defined as

$$s_i = \frac{maxT - T_i}{maxT - minT} \tag{12}$$

T_i is calculated using the raw T1w/T2w value. The self-coupling heterogeneity strength is defined as

$$w_i = w_{min} + w_{scale} s_i \tag{13}$$

where w_{min} and w_{scale} are heterogeneity parameters.

C Synaptic Dynamical Equations

We introduce the biophysically-based computational model to simulate the functional dynamics $\dot{y}_i(t)$ for each node i with the heterogeneity map s_i.

$$\dot{y}_i(t) = -y_i(t) + \sum_j C_{ij} y_j(t) + n_{\nu_i}(t), \tag{14}$$

where $\nu_i(t)$ is the independent Gaussian white noise. C represents the coupling matrix. $y_i(t)$ is the learned representation using the proposed method.

We incorporate the structural connectivity matrix S^C and global coupling parameter G^C with $\dot{y}_i(t)$,

$$\dot{y}_i(t) = -\sum_j [(1 - w_i)\delta_{ij} - G^C S^C_{ij}] y_j(t) + n_{\nu_i}(t), \tag{15}$$

The system's Jacobian matrix is defined as

$$J_{ij} = -[(1 - w_i)\delta_{ij} - G^C S_{ij}^C] \tag{16}$$

The noise term $\nu_i(t)$ is independent and normally distributed with the noise covariance matrix $Q_n = \sigma^2 I$. The covariance matrix could be obtained using the Lyapunov equation

$$JP + PJ^T + Q_n = 0 \tag{17}$$

Then, we could get the functional connectivity as follows,

$$P^{FC} = KPK^\dagger \tag{18}$$

where k is the matrix of partial derivates.

$$FC_{ij} = \frac{P_{ij}^{FC}}{\sqrt{P_i^{FC} P_j^{FC}}} \tag{19}$$

D Within and Across network fitting

We quantify the difference between the proposed heterogeneous graph transformer model and homogeneous model using the following equation,

$$r_N = r_p(FC_{ij}^1, FC_{ij}^2) \tag{20}$$